Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

The Reaction of Acetaldehyde, Glyoxal, and Ammonia to Yield 2-Methylimidazole: Thermodynamic and Kinetic Analyses of the Mechanism

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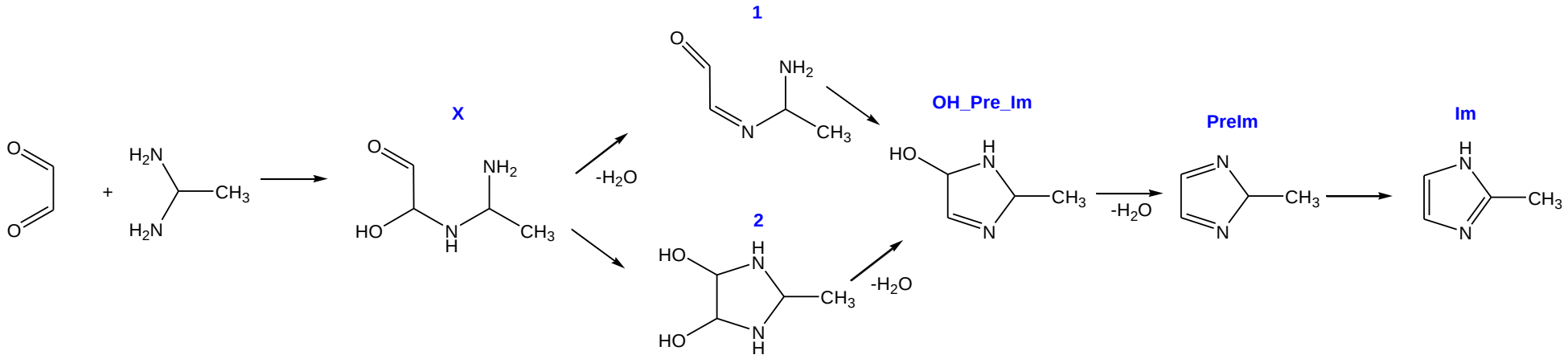
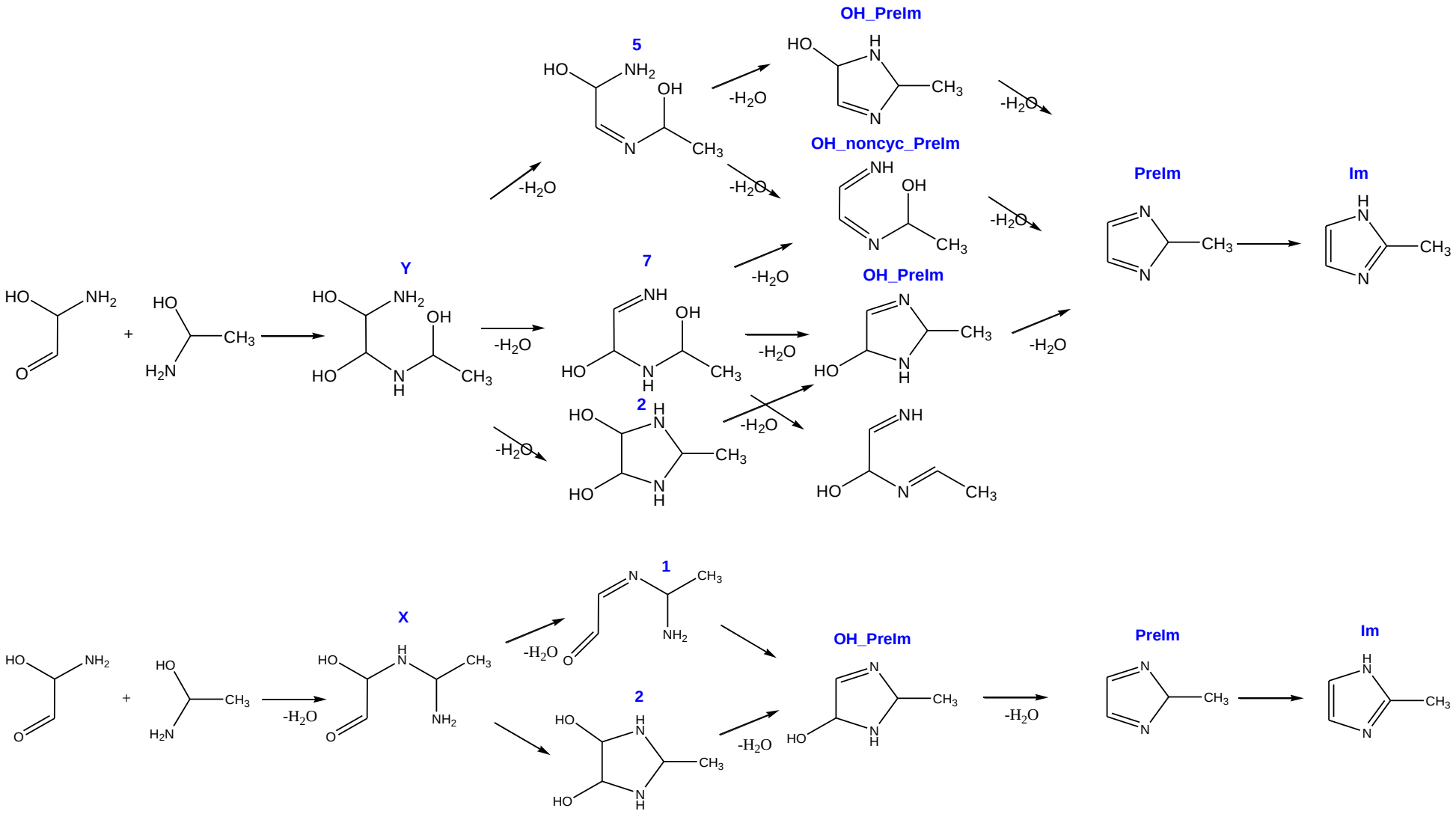
Schemes for the 2-methylimidazole formation

Scheme A



Scheme B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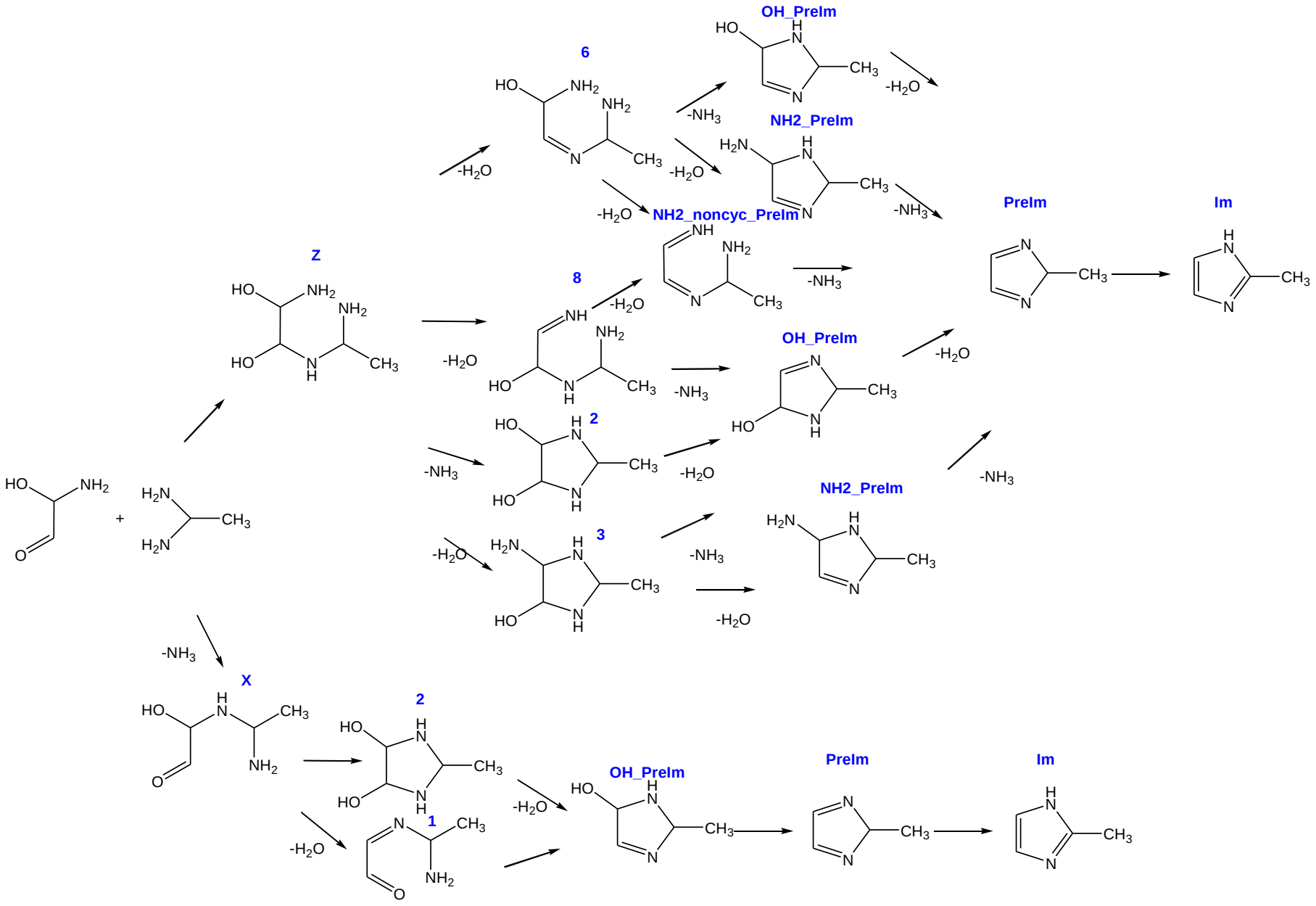
5
OH_noncyc_PreIm
PreIm
Im
Y
7
OH_PreIm
2
X
1
OH_PreIm
2
PreIm
Im
-H2O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NH2_PreIm
NH2_noncyc_PreIm
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Im
Z
8
OH_PreIm
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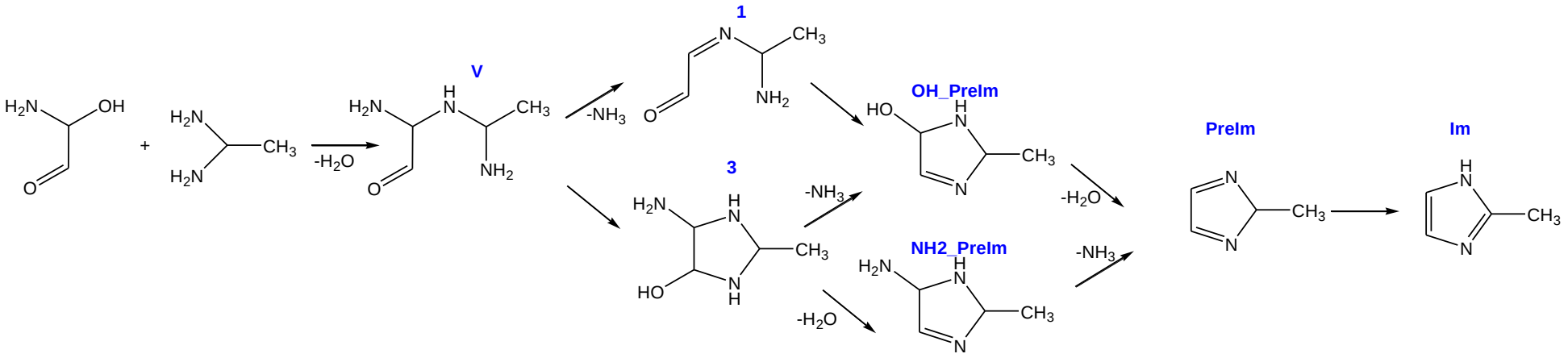
3
X
2
1
OH_PreIm
PreIm
Im


V
1
3
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NH2_PreIm
PreIm
Im
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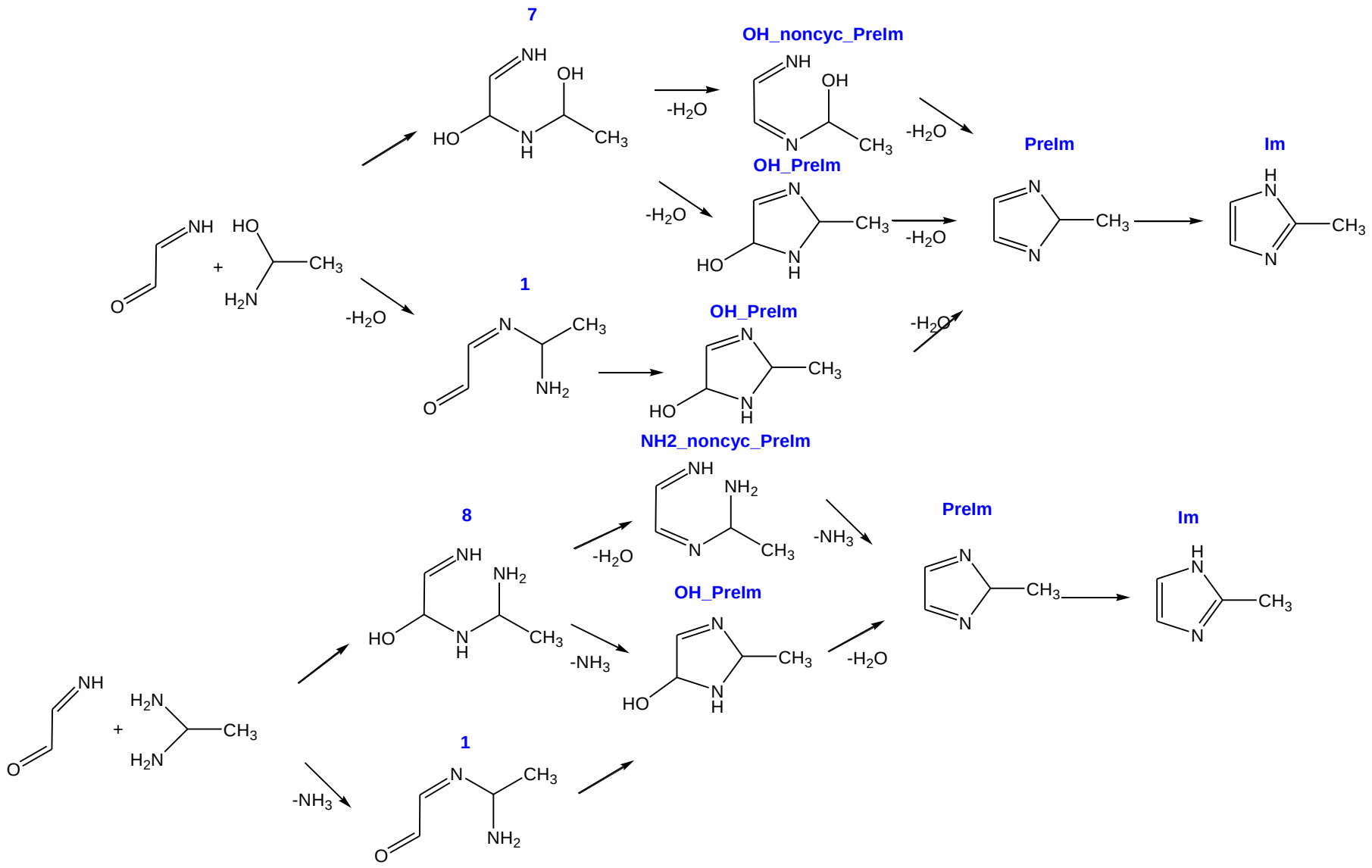
-H2O
-NH3
-H2O
-NH3
-H2O

Scheme C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-H2O
PreIm
Im
OH_PreIm
-H2O
-H2O
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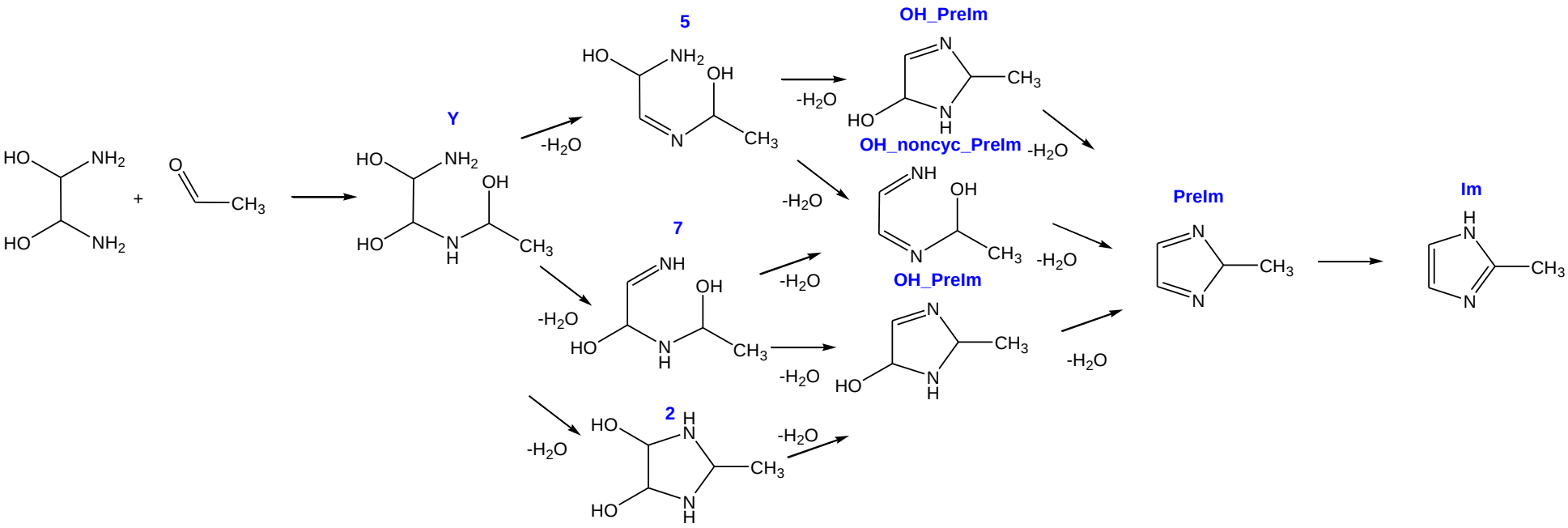
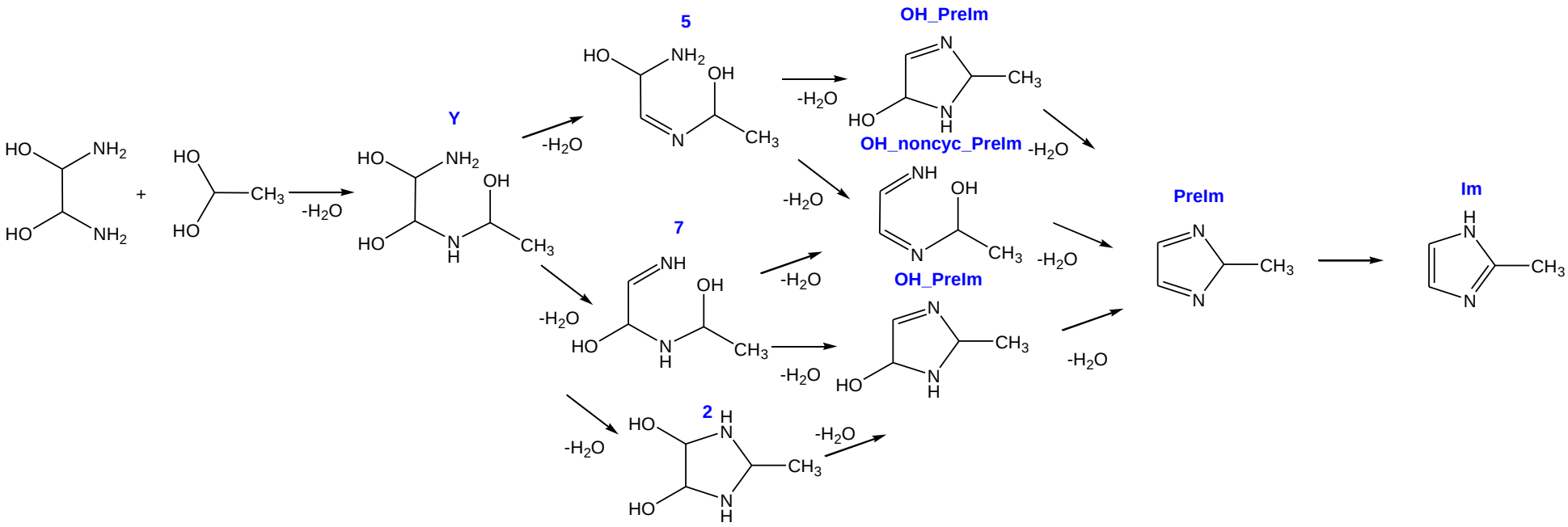
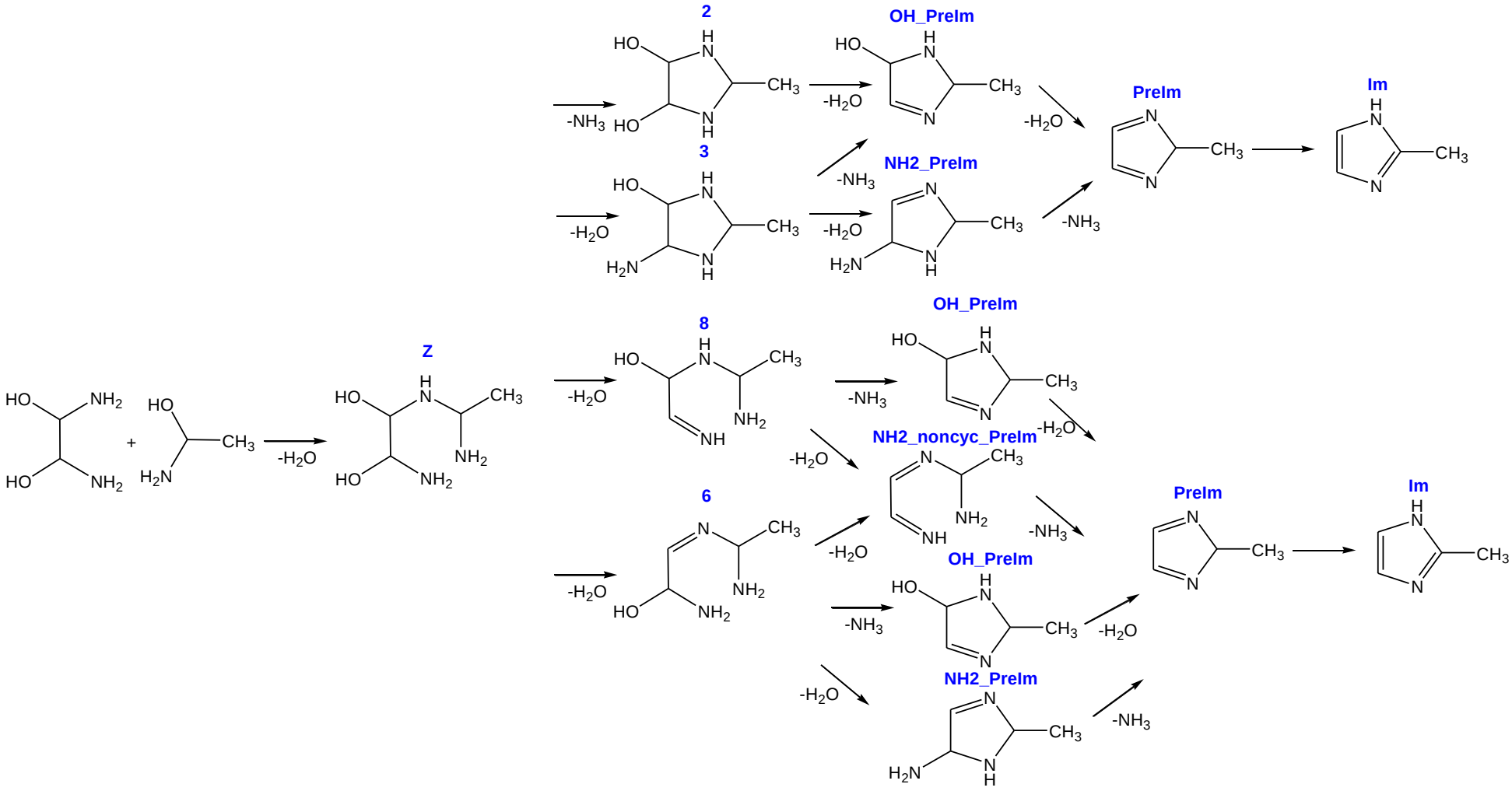
OH_PreIm
-H2O
NH2_noncyc_PreIm
8
-H2O
-NH3
PreIm
Im
OH_PreIm
-NH3
-H2O
-NH3
1

Scheme D




Y
5
7
2
OH_PreIm
OH_noncyc_PreIm
OH_PreIm
PreIm
Im
-H2O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3
NH2_PreIm
PreIm
Im
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NH2_noncyc_PreIm
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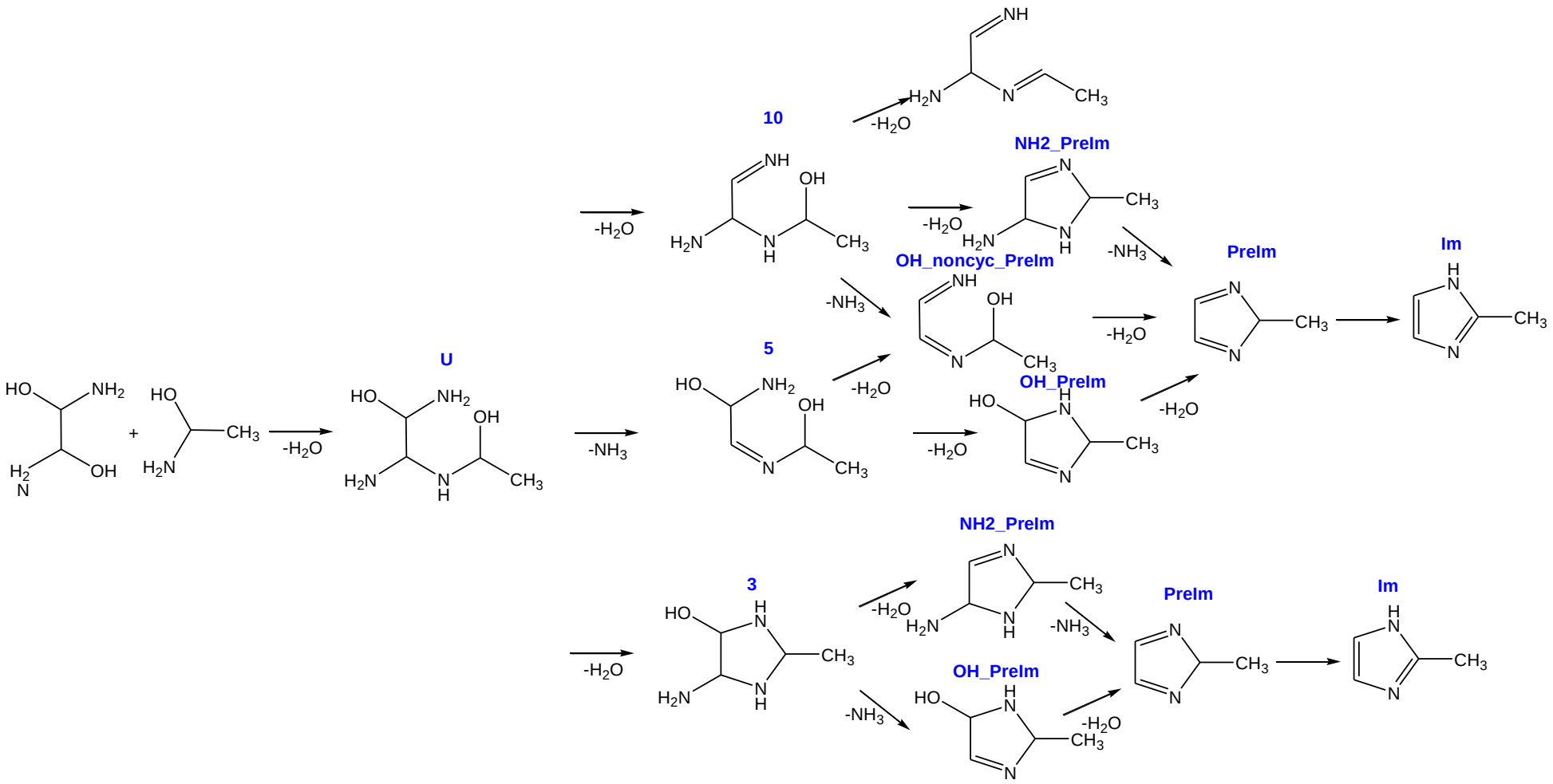
NH2_PreIm
PreIm
Im
-NH3
-H2O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10
5
3
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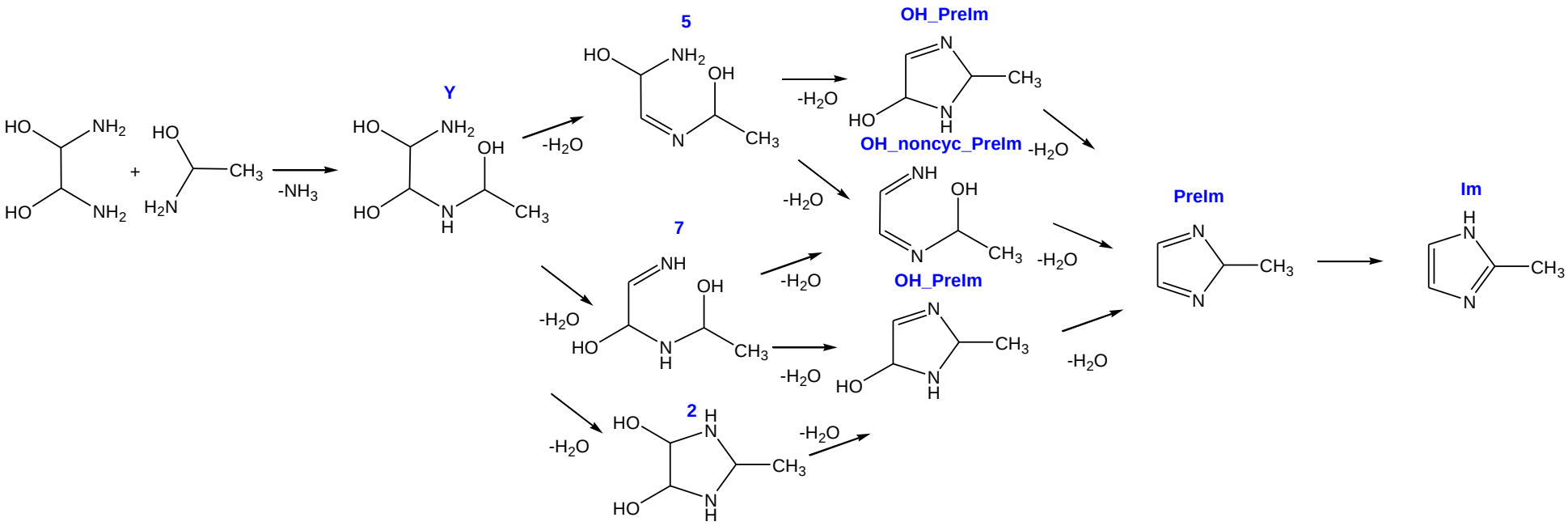
OH_noncyc_Prelm
OH_Prelm
Prelm
Im
-H2O
-NH3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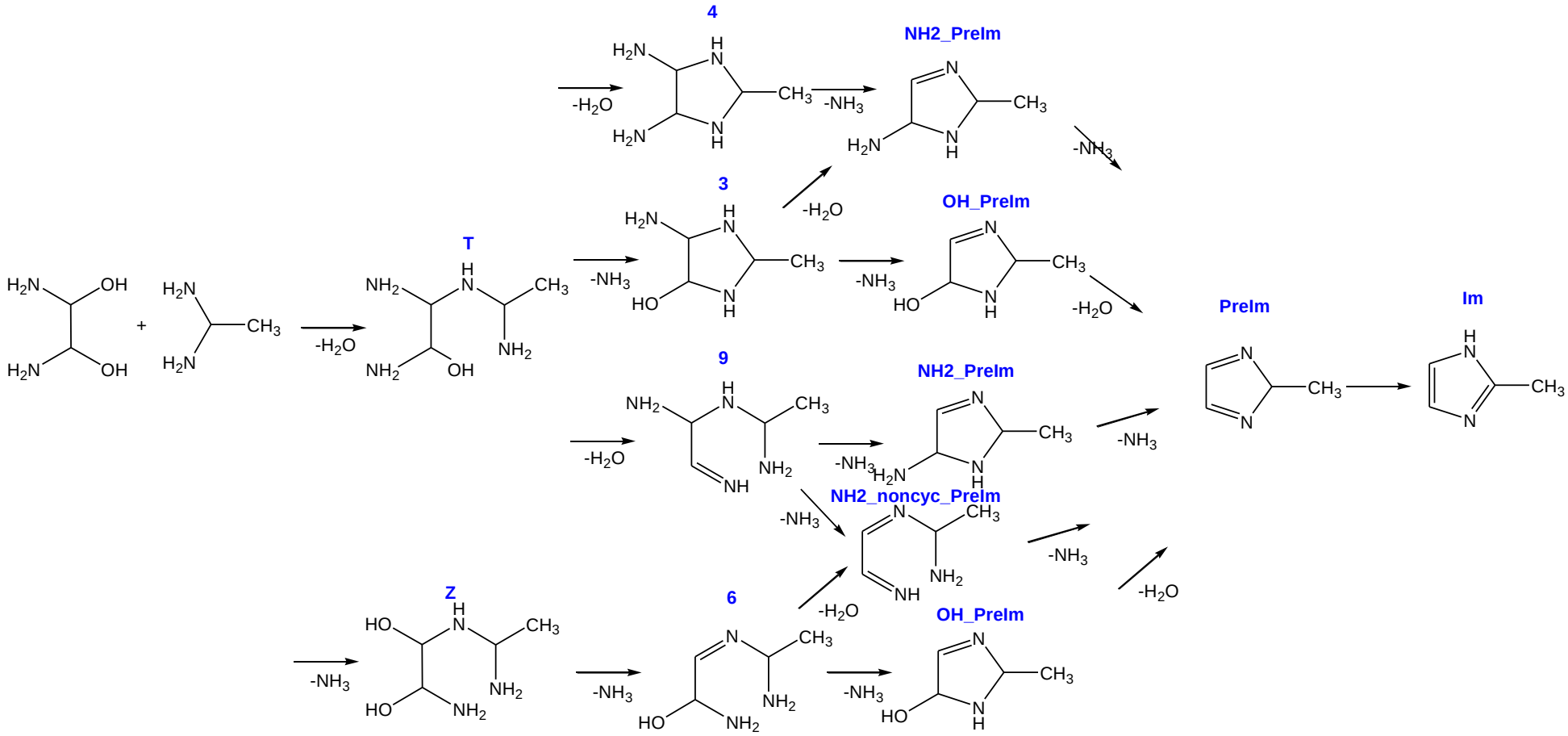
5
OH_PreIm
OH_noncyc_PreIm
7
OH_PreIm
2
PreIm
Im
-NH3
-H2O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NH2_PreIm
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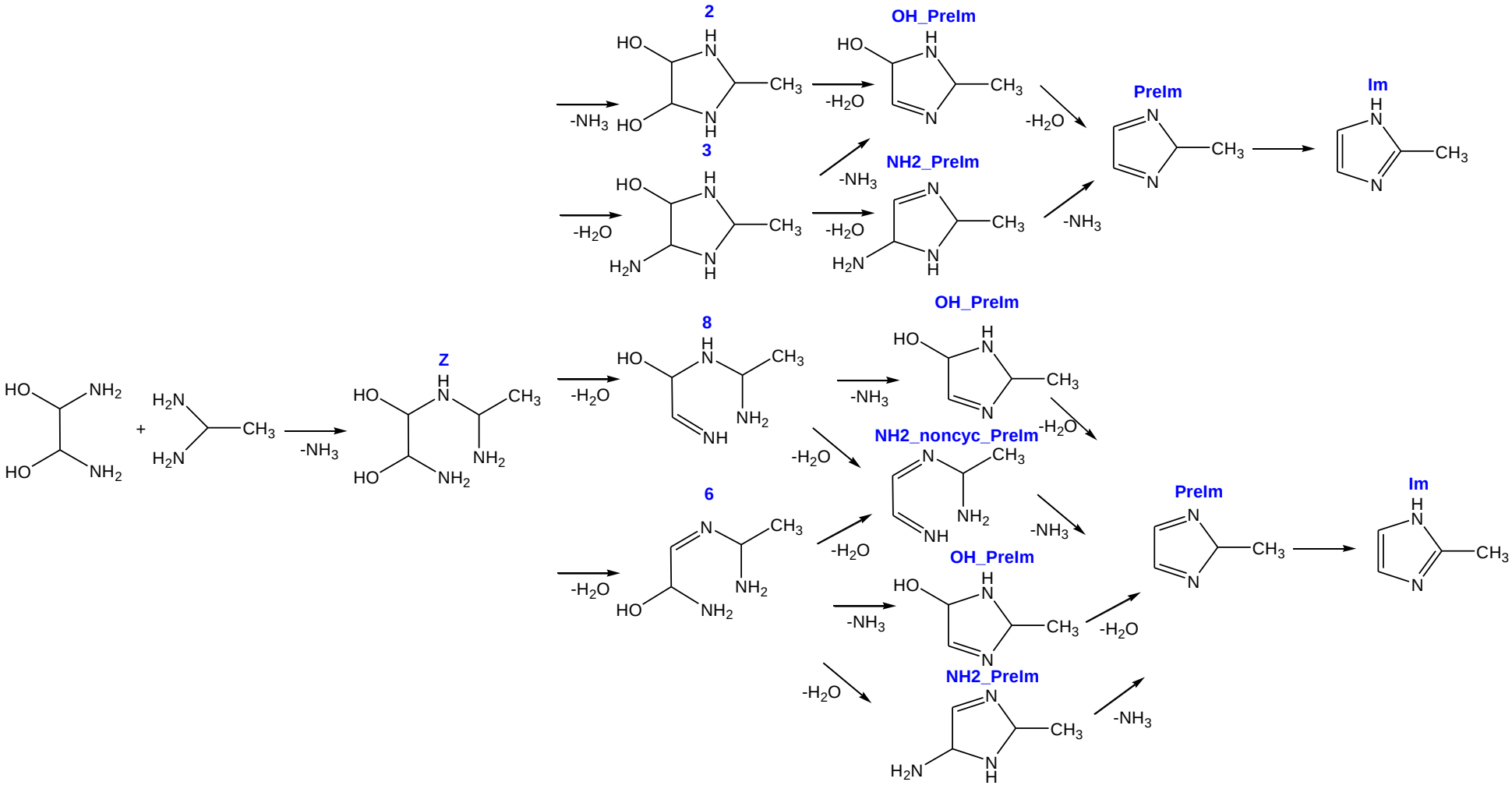
OH_PreIm
T
PreIm
Im
9
NH2_PreIm
NH2_noncyc_PreIm
Z
6
OH_PreIm
-H2O
-NH3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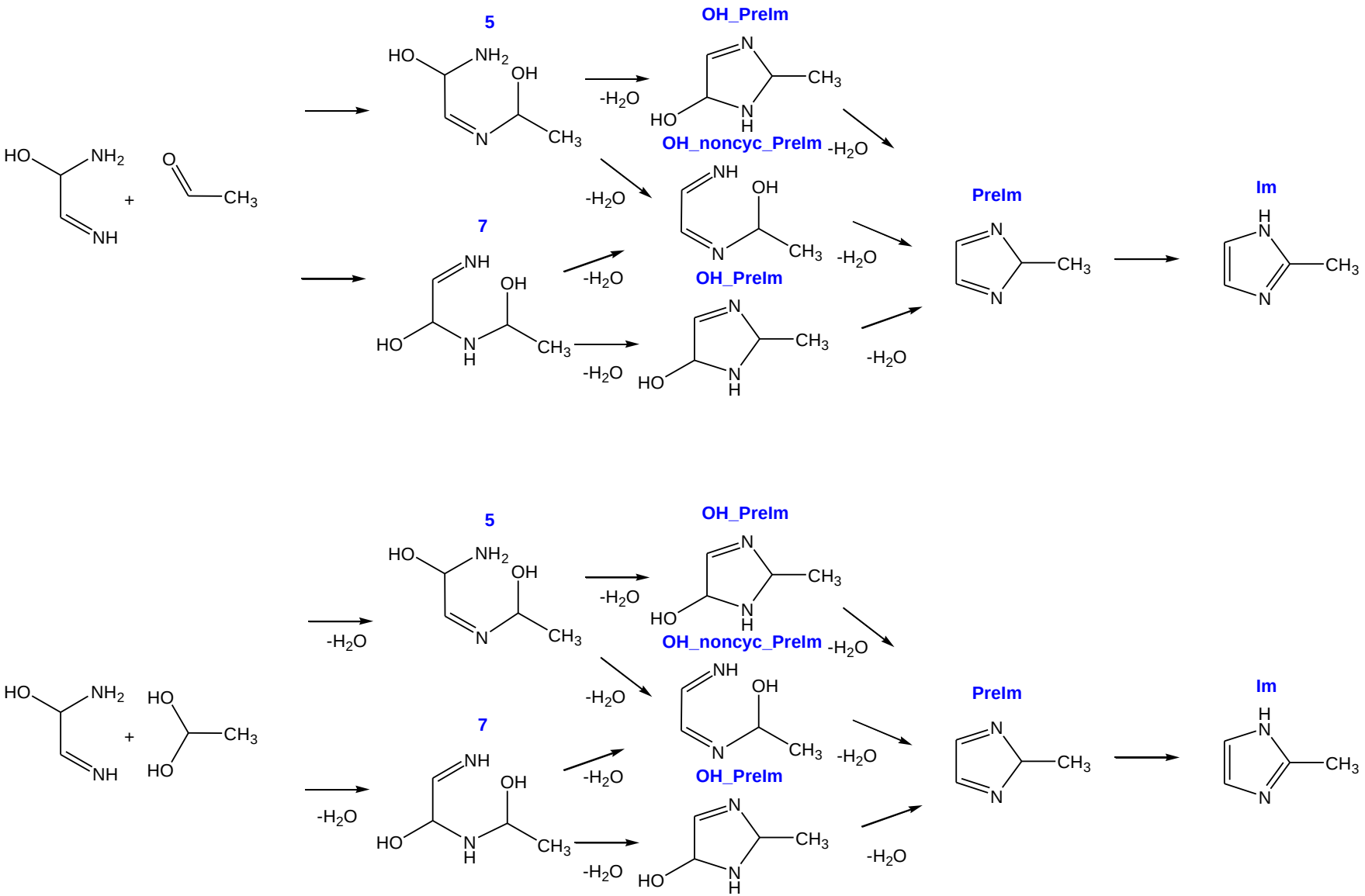
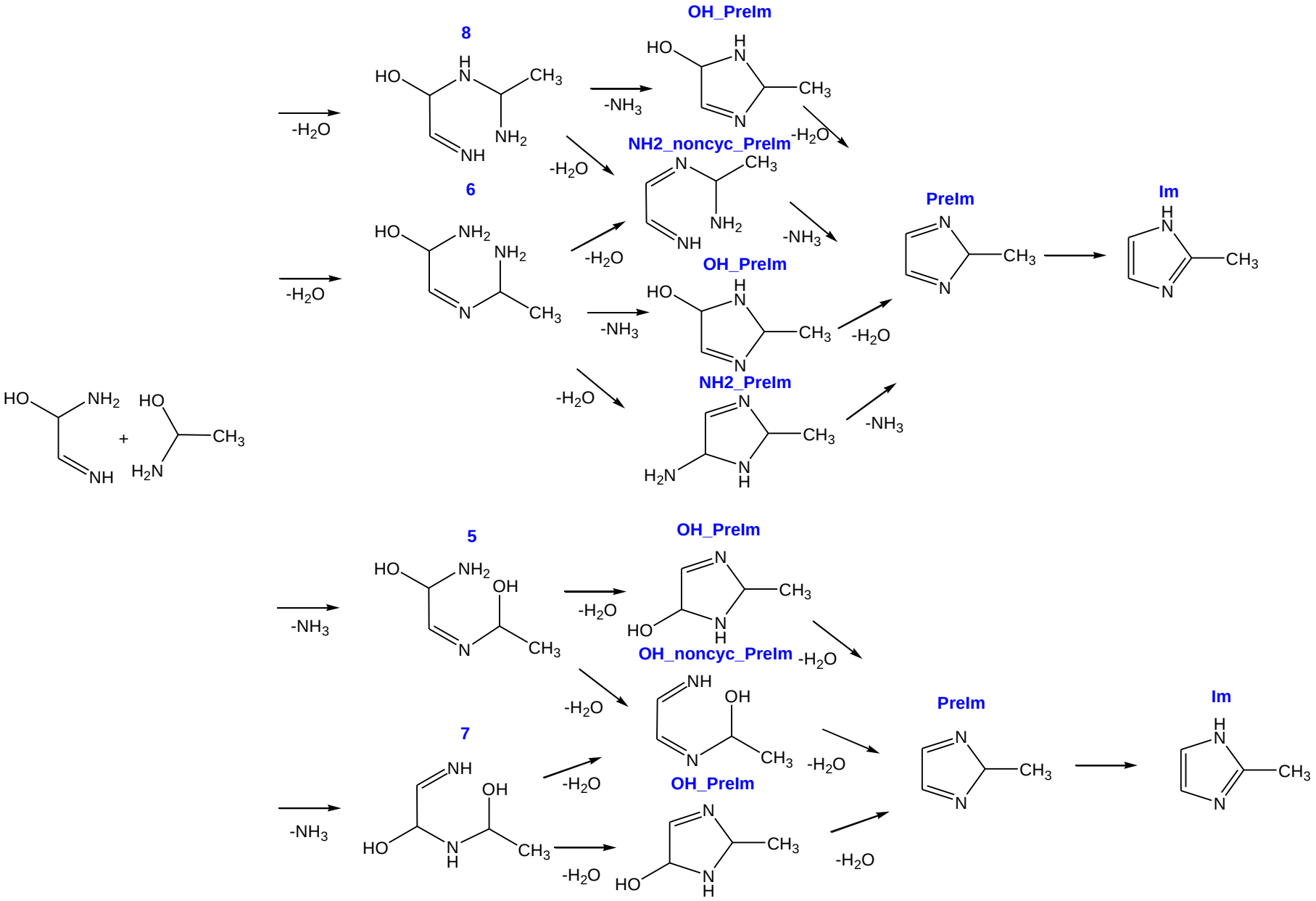
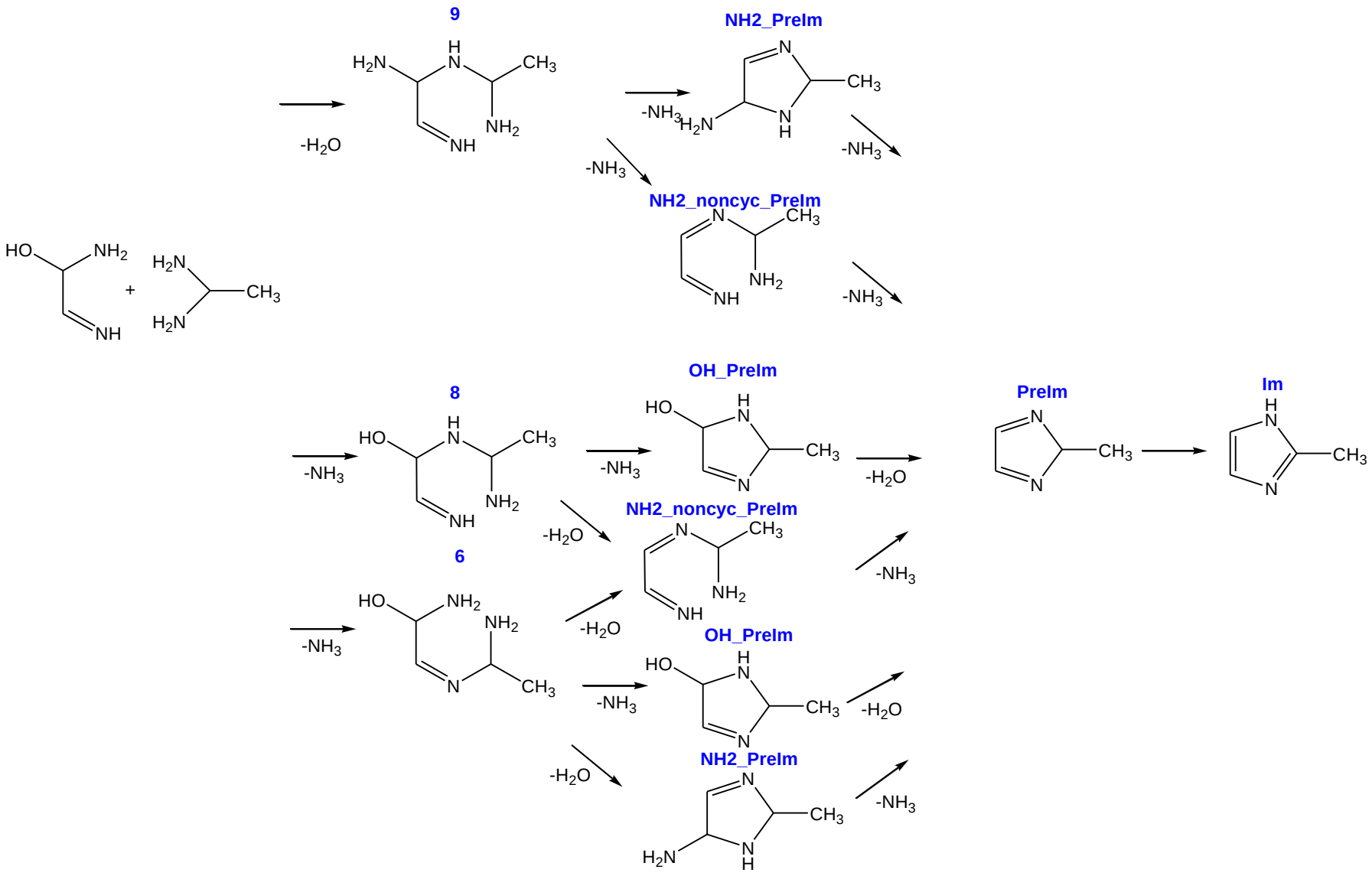
OH_PreIm
3
NH2_PreIm
PreIm
Im
Z
8
OH_PreIm
NH2_noncyc_PreIm
6
OH_PreIm
NH2_PreIm
PreIm
Im

Scheme E




8
OH_PreIm
-H2O
-NH3
-H2O
NH2_noncyc_PreIm
6
-H2O
-NH3
PreIm
Im
-H2O
OH_PreIm
-NH3
-H2O
NH2_PreIm
-H2O
-NH3
5
OH_PreIm
-NH3
-H2O
OH_noncyc_PreIm
-H2O
7
-H2O
-H2O
PreIm
Im
-NH3
OH_PreIm
-H2O
-H2O


9
NH2_PreIm
-H2O
-NH3
-NH3
-NH3
NH2_noncyc_PreIm
-NH3
OH_PreIm
8
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-NH3
-H2O
NH2_noncyc_PreIm
6
-NH3
-H2O
-NH3
OH_PreIm
-H2O
-NH3
NH2_PreIm
PreIm
Im

Scheme F

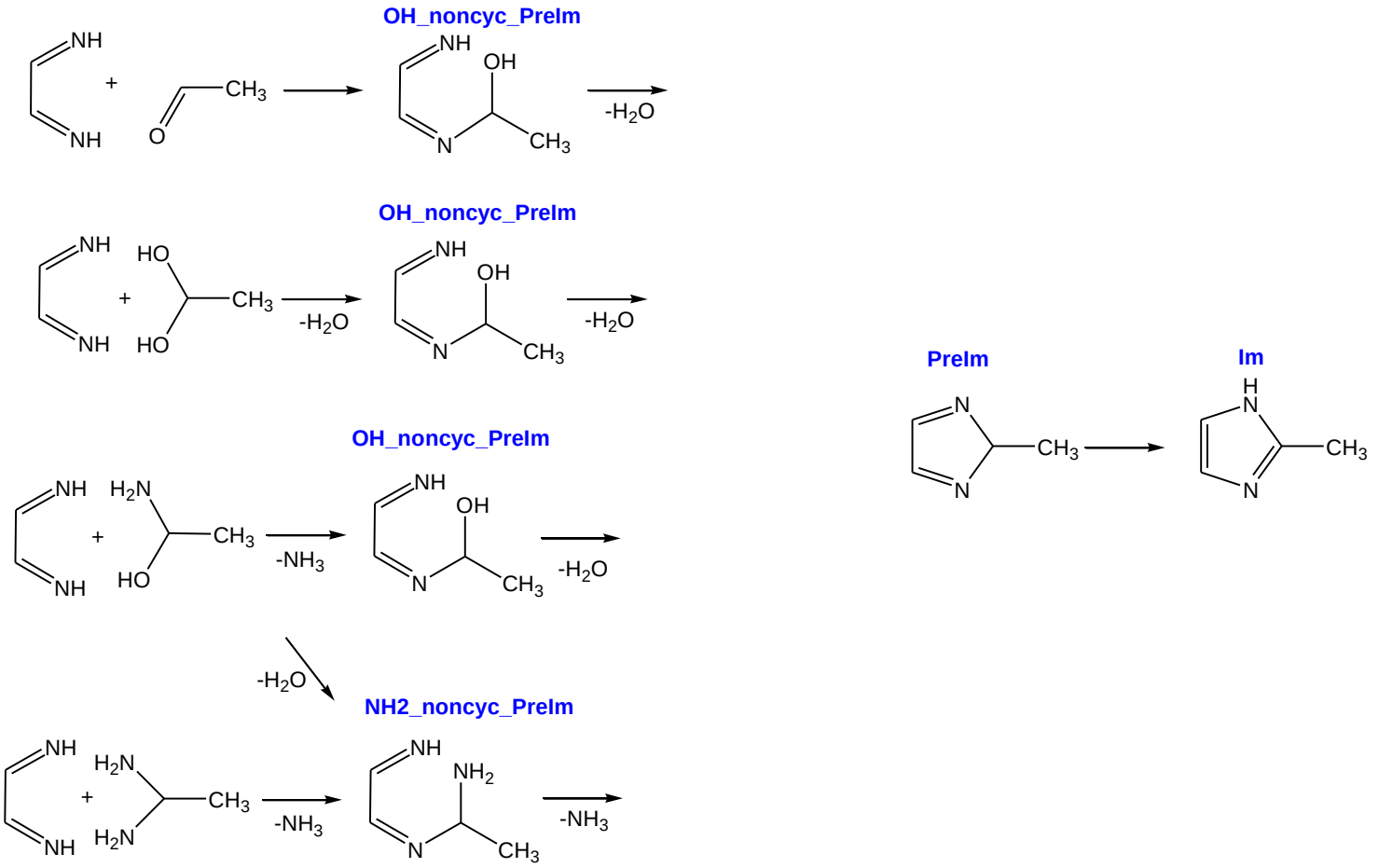

OH_noncyc_PreIm
OH_noncyc_PreIm
OH_noncyc_PreIm
NH2_noncyc_PreIm
-H2O
-NH3
PreIm
Im

Table S1. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme A).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
X	-418.397340	-262548.31	-4.7
1.	-341.941343	-214571.44	5.7
2.	-418.394693	-262546.64	-3.1
OH_Pre_Im	-341.953040	-214578.78	-1.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S2. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme B).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Bt_OHC-CHOHNH2	-284.442632	-178490.45	-5.7
Bc_OHC-CHOHNH2	-284.440698	-178489.24	-4.5
Y	-494.845299	-310520.13	-10.1
X	-418.397340	-262548.31	-4.7
Z	-474.956671	-298039.82	-8.0
V	-398.507532	-250067.26	-1.9
5	-418.393549	-262545.93	-2.3
7	-418.386432	-262541.46	2.1
2	-418.394693	-262546.64	-3.1
OH_PreIm	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.94197	-214571.83	5.3
1	-341.941343	-214571.44	5.7
6	-398.502137	-250063.88	1.5
8	-398.497186	-250060.77	4.6
3	-398.505197	-250065.80	-0.5

NH2_PreIm	-322.067231	-202100.25	-1.4
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S3. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme C).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Cc_OHC-CHNH	-207.993268	-130517.75	0.5
Ct_OHC-CHNH	-207.991031	-130516.35	1.9
1	-341.941343	-214571.44	5.7
7	-418.386432	-262541.46	2.1
8	-398.497186	-250060.77	4.6
OH_Pre_Im	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S4. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme D).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Dc_NH2HOHC-CHOHNH2	-341.006158	-213984.60	-11.7
Dt_NH2HOHC-CHOHNH3	-340.998213	-213979.62	-6.7
Y	-494.845299	-310520.13	-10.1
Z	-474.956671	-298039.82	-8.0
U	-474.958099	-298040.72	-8.9
W	-455.066935	-285558.82	-5.3
2.	-418.394693	-262546.64	-3.1

3.	-398.505197	-250065.80	-0.5
4.	-378.622770	-237589.39	-2.3
5.	-418.393549	-262545.93	-2.3
6.	-398.502137	-250063.88	1.5
7.	-418.386432	-262541.46	2.1
8.	-398.497186	-250060.77	4.6
9.	-378.613817	-237583.77	3.3
10.	-398.501704	-250063.61	1.7
OH_Pre_Im	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_PreIm	-322.067231	-202100.25	-1.4
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S5. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme E).

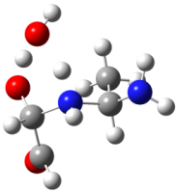
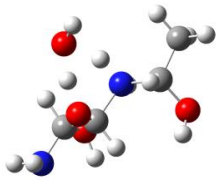
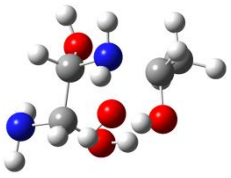
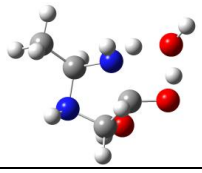
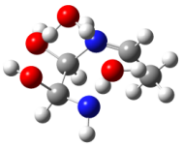
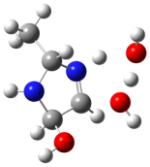
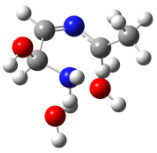
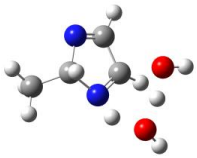
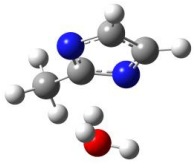
Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0
Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
1.1-diaminoethane	-190.513636	-119549.12	3.8
Ec_NH2HOHC-CHNH	-264.549056	-166007.05	-0.6
Et_NH2HOHC-CHNH	-264.545815	-166005.01	1.4
5.	-418.393549	-262545.93	-2.3
6.	-398.502137	-250063.88	1.5
7.	-418.386432	-262541.46	2.1
8.	-398.497186	-250060.77	4.6
9.	-378.613817	-237583.77	3.3
OH_PreIm	-341.953040	-214578.78	-1.7
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_PreIm	-322.067231	-202100.25	-1.4
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S6. The Gibbs free energies of the structures in solution and the PES positions of all structures of the proposed mechanism of 2-methylimidazole formation (Scheme F).

Structure	G, a.u.	G, kcal/mol	Gposition
trans-Glyoxal (trans-GO)	-227.879412	-142996.50	0.0
Water	-76.448667	-47972.26	0.0
Ammonia	-56.563306	-35494.01	0.0

Acetaldehyde	-153.850943	-96542.93	0.0
cis-Glyoxal (cis-GO)	-227.875282	-142993.90	2.6
1.1-ethanediol	-230.291459	-144510.08	-1.1
1-aminoethanol	-210.403067	-132029.92	1.2
ethanimine	-133.954955	-84058.01	6.7
Fc_HNHC-CHNH	-188.099923	-118034.49	5.5
Ft_HNHC-CHNH	-188.102608	-118036.17	3.8
OH_non_cyc_PreIm	-341.941977	-214571.84	5.3
NH2_non_cyc_PreIm	-322.051200	-202090.19	8.7
PreIm	-265.518264	-166615.23	-4.6
Im	-265.552189	-166636.52	-25.9

Table S7. Transition states with the participation of one water molecule, and their Gibbs free energies and stage barriers for the mechanism of 2-methylimidazole formation

Reagents, TSs, products	TS	G, a.u	G, kcal/mol	$\Delta G^{\#}$, kcal/mol
cis-Glyoxal		-227.875282	-142993.9	
1.1-diaminoethane		-190.513636	-119549.1	
Water		-76.448667	-47972.3	
GO+NH2NH2CHCH3_X		-494.820826	-310504.8	3.0
X		-418.39734	-262548.3	
Bc_OHC-CHOHNH2		-284.440698	-178489.2	
Water		-76.448667	-47972.3	
1-aminoethanol		-210.403067	-132029.9	
Bc+OHNH2CHCH3_Y		-571.275241	-358480.6	3.3
Y		-494.845299	-310520.1	
Dc_NH2HOHC-CHOHNH2		-341.006158	-213984.6	
Acetaldehyde		-153.850943	-96542.9	
Water		-76.448667	-47972.3	
Dc_Y		-571.272646	-358479.0	13.3
Y		-494.845299	-310520.1	
X		-418.39734	-262548.3	
Water		-76.448667	-47972.3	
X_2		-494.82611	-310508.1	5.0
2		-418.394693	-262546.6	
Y		-494.845299	-310520.1	
Water		-76.448667	-47972.3	
Y_2		-571.244764	-406413.6	23.4
2		-418.394693	-262546.6	
2		-418.394693	-262546.6	
Water		-76.448667	-47972.3	
2_OH_PreIm		-494.802258	-310493.1	18.3
OH_PreIm		-341.953040	-214578.8	
5		-418.393549	-262545.9	
Water		-76.448667	-47972.3	
5_OH_PreIm		-571.228823	-358451.5	31.4
OH_PreIm		-341.953040	-214578.8	
OH_PreIm		-341.953040	-214578.8	
Water		-76.448667	-47972.3	
OH_PreIm_PreIm		-418.368062	-262529.9	13.6
PreIm		-265.518264	-166615.2	
PreIm		-265.518264	-166615.2	
Water		-76.448667	-47972.3	
PreIm_2MI		-341.921864	-214559.2	20.8
2MI		-265.552189	-166636.5	

Identification of ^{1}H NMR signals in the spectra of reaction mixtures of 2MI formation with different orders of mixing of reagents

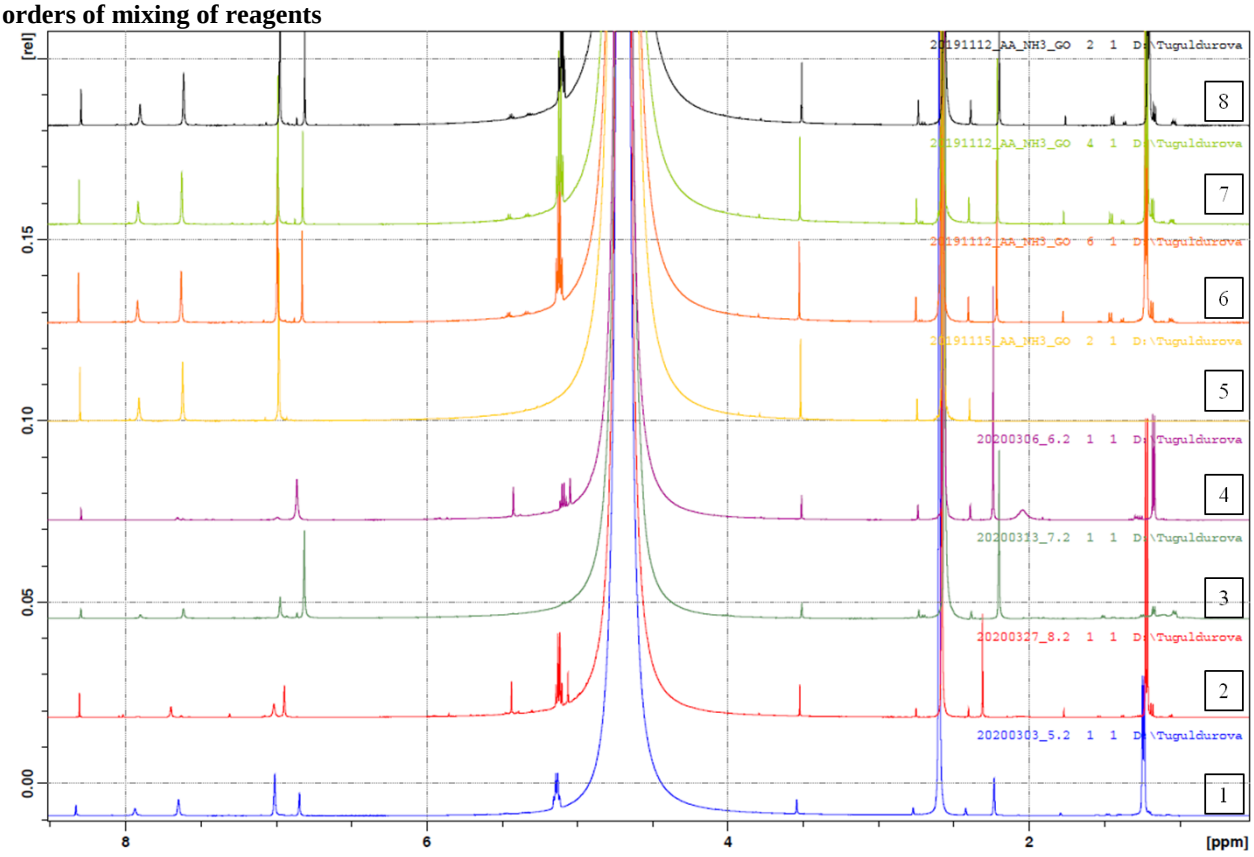


Fig. S1. ^{1}H NMR spectra of reaction mixtures of 2MI formation with different orders of mixing of reagents. The internal standard was DMSO.
1 (blue) - Acetaldehyde → Glyoxal → Ammonia
2 (red) - Glyoxal → Ammonia → Acetaldehyde
3 (green) - Acetaldehyde → Ammonia → Glyoxal
4 (purple) - Water → Glyoxal → Ammonia
5 (yellow) - Water → lack of THT → Glyoxal
6 (orange) Water → THT → Ammonia → Glyoxal
7 (light green) - Acetaldehyde → lack of ammonia (3 h, 10 °C) → Glyoxal
8 (black) - Acetaldehyde → Ammonia (3 h, 10 °C) → Glyoxal

Figure S1 shows the ^{1}H NMR spectra of the reaction mixtures of 2MI formation with different orders of mixing of the reagents at the end of the reaction. The chemical shift of the singlet signal of the protons of the internal standard (DMSO) is located in the region of 2.58 ppm. The protons of the methyl group of acetaldehyde feature a chemical shift of 1.22 ppm. The singlet of the protons of the methyl substituent in 2MI is detected at 2.21 ppm, and the signals of the methine protons of the imidazole ring of 2MI appear in a weak field (6.83 ppm). The spectral pattern of the reaction mixtures indicates the presence of additional signals in the regions of 3.53 ppm, 6.99 ppm, 7.63 ppm, 7.92 ppm, and 8.313 ppm, and these signals are related to the products of the competing reaction of glyoxal with ammonia. Singlet signal at 3.53 ppm is assigned to the protons of the CH_2 group of glycolic acid formed as a result of the Cannizzaro reaction, which was shown in our previous work[30]. The signal at 6.99 ppm can be reliably assigned to the methine protons of the imidazole ring of hydrated imidazole-2-carbocaldehyde (HIC) since Ref.[32] shows that similar protons of unhydrated imidazole-2-carbaldehyde (IC) appear in at 7.47 ppm. The 0.5 ppm shift is connected with the deactivation of the methine protons of the ring by the carbonyl group, which is characterized by a negative mesomeric effect that leads to a downfield shift of the signal, which is not observed in the case of the hydrated product. The remaining three signals in the weak field remain unidentified.

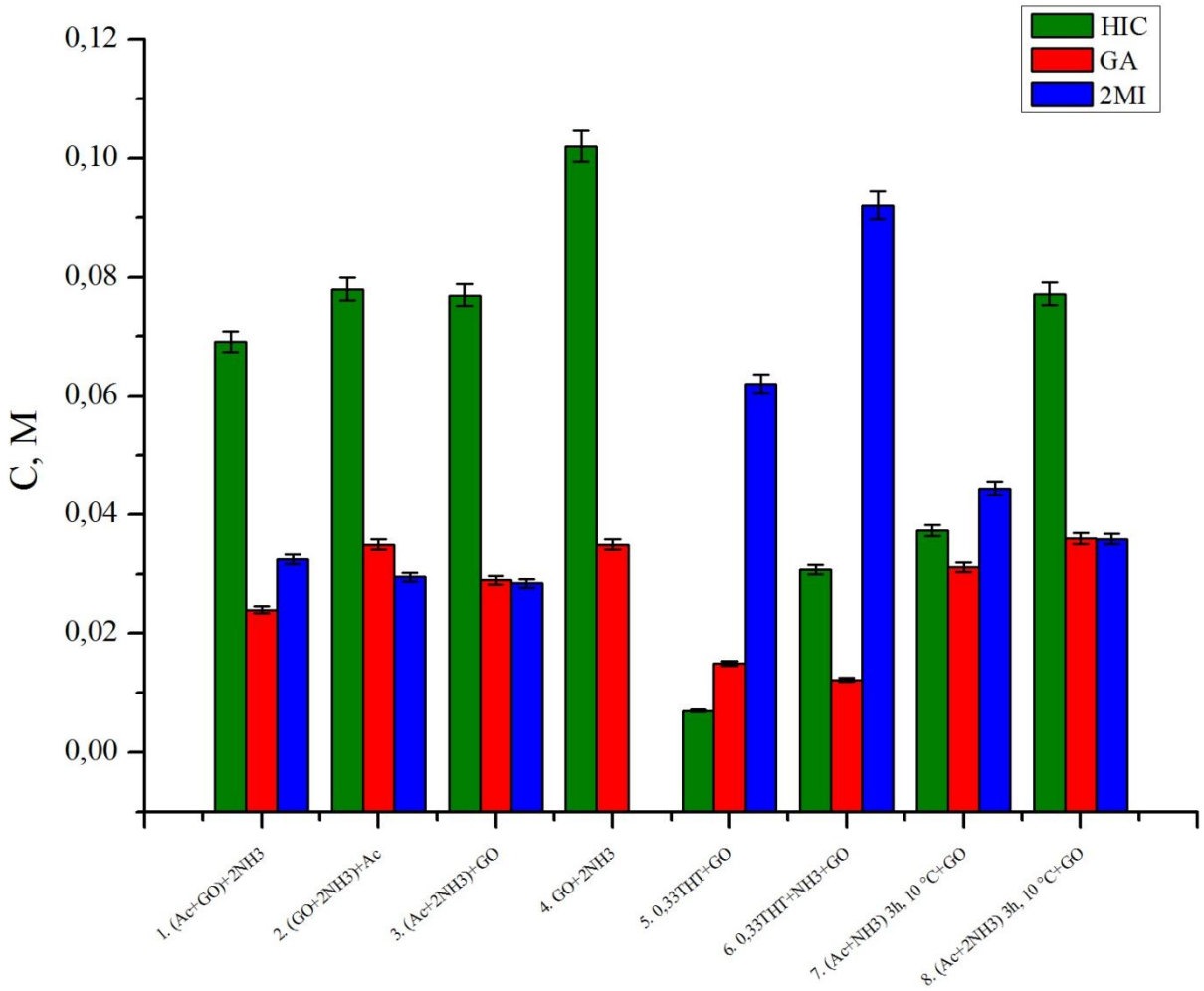


Fig. S2. Concentrations of the main products of the interaction of acetaldehyde, glyoxal, and ammonia in aqueous solution depending on the order of reagent mixing

Table S8. Concentrations of the main products, glyoxal conversion and selectivities towards the main products of the interaction of acetaldehyde, glyoxal, and ammonia in aqueous solution depending on the order of reagent mixing

No.	Order of reagent mixing and their molar ratios	C(HIC),M	C(GA), M	C(2MI), M	Total yield[1], M	Selectivity[2], %			GO Conversion[3], %
						HIC	**GA**	**2MI**	
1	(Ac+GO)+2NH_3	0.069	0.024	0.033	0.195	70.8	12.3	16.9	58.6
2	(GO+2NH_3)+Ac	0.078	0.035	0.03	0.221	70.6	15.8	13.6	66.4
3	(Ac+2NH_3)+GO	0.077	0.029	0.029	0.212	72.6	13.7	13.7	63.7
4	GO+2NH_3	0.102	0.035		0.239	85.4	14.6	0.0	71.8
5	0.33THT+GO	0.007	0.015	0.062	0.091	15.4	16.5	68.1	27.3
6	0.33THT+NH_3+GO	0.031	0.012	0.092	0.166	37.3	7.2	55.4	49.8
7	(Ac+NH_3)10 °C, 3h +GO	0.037	0.031	0.044	0.149	49.7	20.8	29.5	44.7
8	(Ac+2NH_3)10 °C, 3h +GO	0.077	0.036	0.036	0.226	68.1	15.9	15.9	67.9

[1]Total yield = **2**·C(HIC)+C(GA)+C(2MI). **2** are because HIC formation requires 2 mol GO.

[2] $Selectivity = \frac{C_i}{Total\ yield} * 100.\%$. The concentration was multiplied by 2 in the case of HIC.

[3] $Conversion = \frac{Total\ yield}{C(GO)_{initial}} * 100.\%$

Table S9. Cartesian coordinates of the most stable states for all structures

Structure	Atom	X	Y	Z
trans-Glyoxal (trans-GO)	C	0.3291	0.6898	0.0000
	O	-0.3291	1.6986	-0.0001
	H	1.4356	0.6728	0.0001
	C	-0.3291	-0.6898	0.0000
	O	0.3291	-1.6986	-0.0001
	H	-1.4356	-0.6728	0.0001
Water	O	0.0682	0.2921	-0.0000
	H	0.8072	-0.2921	-0.0000
	H	-0.8072	-0.0559	0.0000
Ammonia	N	-0.0026	0.2314	-0.2007
	H	-0.8094	0.7032	0.2006
	H	0.8094	0.6942	0.2006
	H	-0.0078	-0.7032	0.2007
Acetaldehyde	C	0.4646	0.2646	-0.0006
	H	0.5337	1.3728	-0.0001
	O	1.4692	-0.4100	-0.0008
	C	-0.9331	-0.2827	-0.0004
	H	-1.4692	0.0926	-0.8784
	H	-0.9225	-1.3728	-0.0009
	H	-1.4687	0.0918	0.8784
cis-Glyoxal (cis-GO)	C	0.0000	-0.7730	0.0136
	O	0.0000	-1.4018	-1.0120
	H	0.0000	-1.2506	1.0120
	C	0.0000	0.7730	0.0136
	O	0.0000	1.4018	-1.0120
	H	0.0000	1.2506	1.0120
B_c_OHC-CHOHNH$_2$	C	0.8417	-0.4904	0.1442
	O	1.7497	0.0596	-0.4283
	H	0.9531	-1.5070	0.5773
	O	-0.6004	1.3820	-0.1804
	H	-1.5319	1.6270	-0.2366
	N	-1.5234	-0.7741	-0.4390
	H	-1.1693	-1.0217	-1.3586
	H	-1.7497	-1.6270	0.0609
	C	-0.5749	0.0570	0.2934
	H	-0.8437	-0.0080	1.3586
C_c_OHC-CHNH	C	-0.2369	0.3880	0.0000
	H	-0.1424	1.4785	0.0000
	C	1.0481	-0.3784	-0.0001
	O	2.1322	0.1573	0.0001
	H	0.9206	-1.4785	0.0001
	N	-1.3235	-0.2695	0.0000
	H	-2.1322	0.3560	0.0001
E_c_NH$_2$HOHC-CHNH	C	0.5183	-0.0316	0.3327
	H	0.4736	-0.0114	1.4295
	C	-0.8325	-0.0075	-0.3457
	H	-0.6782	-0.0019	-1.4295
	O	-1.4420	1.2181	0.0890
	H	-2.2921	1.2964	-0.3590
	N	1.5921	-0.0723	-0.3388
	H	2.4023	-0.0947	0.2841
	N	-1.5601	-1.2053	0.0041
	H	-1.8415	-1.1706	0.9803
	H	-2.4023	-1.2964	-0.5552
F_c_HNHC-CHNH	C	-0.2922	0.4439	0.0003
	H	-0.7698	1.4286	0.0000
	C	1.2077	0.4398	-0.0003

	H	1.6905	1.4189	-0.0002
	N	-0.9257	-0.6569	0.0000
	H	-1.9345	-0.5022	-0.0002
	N	1.9345	-0.6026	-0.0003
	H	1.3224	-1.4286	-0.0001
D_c_NH_2HOHC-$CHOHNH_2$	C	-0.6299	-0.3627	-0.4534
	H	-0.7285	-1.0530	-1.2997
	C	0.7616	0.2819	-0.5174
	H	0.8624	0.8347	-1.4568
	O	1.6663	-0.8420	-0.5066
	H	2.5645	-0.5002	-0.4413
	O	-0.7423	-1.1070	0.7781
	H	0.0216	-1.6993	0.8067
	N	-1.6500	0.6365	-0.5438
	H	-2.5645	0.2108	-0.4339
	H	-1.5206	1.3091	0.2072
	N	0.9321	1.2023	0.5761
	H	0.8970	0.6985	1.4568
	H	1.8136	1.6993	0.5179
1.1-ethanediol_$HO(HO)CHCH_3$	C	1.2090	-0.0026	-0.2046
	H	1.7077	-0.8925	0.1814
	H	1.7098	0.8863	0.1812
	H	1.2750	-0.0027	-1.2954
	C	-0.2480	-0.0012	0.2015
	H	-0.3538	-0.0011	1.2954
	O	-0.8386	-1.1757	-0.3322
	H	-1.7098	-1.2851	0.0646
	O	-0.8359	1.1742	-0.3321
	H	-1.7072	1.2851	0.0641
1-aminoethanol_$HO(NH_2)CHCH_3$	C	0.1492	0.3461	0.2296
	H	0.1778	0.3934	1.3265
	O	0.6581	1.6146	-0.1785
	H	0.7728	1.5579	-1.1363
	N	1.0052	-0.6958	-0.3269
	H	1.9085	-0.6813	0.1376
	H	0.6033	-1.6146	-0.1669
	C	-1.2899	0.1432	-0.2335
	H	-1.7069	-0.7869	0.1630
	H	-1.9085	0.9750	0.1071
	H	-1.3237	0.1016	-1.3265
Ethanimine_$NHCHCH_3$	N	-1.5271	-0.3007	-0.0005
	H	-1.3822	-1.3157	-0.0007
	C	-0.4068	0.3003	-0.0003
	H	-0.4346	1.3953	-0.0001
	C	0.9688	-0.3034	-0.0002
	H	1.5271	0.0370	-0.8785
	H	1.5267	0.0362	0.8785
	H	0.9321	-1.3953	-0.0008
1.1-diaminoethane_$NH_2(NH_2)CHCH_3$	C	0.2556	-0.0234	0.2282
	H	0.2685	-0.0413	1.3297
	N	1.1016	-1.1415	-0.2054
	H	0.7466	-2.0079	0.1902
	H	1.0235	-1.2322	-1.2167
	N	0.8584	1.1959	-0.3221
	H	0.3264	2.0079	-0.0224
	H	1.7927	1.3015	0.0640
	C	-1.2017	-0.1148	-0.2360
	H	-1.6605	-1.0365	0.1306
	H	-1.7927	0.7297	0.1336
	H	-1.2426	-0.1125	-1.3297

X	C	-2.3682	-0.8639	-0.0349
	C	-1.6911	0.4194	-0.5350
	C	0.6069	-0.1981	0.0427
	H	-2.6094	-0.8585	1.0434
	H	-2.2736	0.7684	-1.3959
	N	-0.3520	0.1608	-1.0089
	C	1.9989	-0.3528	-0.5710
	H	2.7145	-0.6510	0.1986
	H	1.9815	-1.1179	-1.3526
	H	2.3458	0.5868	-1.0122
	H	0.6414	0.5710	0.8253
	O	-1.7970	1.3462	0.5518
	H	-0.0115	0.9414	-1.5601
	H	-1.5101	2.2098	0.2354
	N	0.0777	-1.4007	0.6823
	H	0.2028	-2.2098	0.0792
	H	0.5514	-1.5840	1.5601
	O	-2.7145	-1.7515	-0.7799
V	C	-2.3550	-0.9245	-0.0208
	C	-1.7023	0.3764	-0.5204
	C	0.6138	-0.2458	0.0551
	H	-2.5540	-0.9549	1.0673
	H	-2.2755	0.6638	-1.4134
	N	-0.3471	0.1163	-0.9916
	C	2.0089	-0.3612	-0.5629
	H	2.7295	-0.6723	0.1968
	H	2.0030	-1.1020	-1.3680
	H	2.3420	0.5965	-0.9752
	H	0.6370	0.4999	0.8599
	H	-0.0101	0.9106	-1.5256
	N	0.1093	-1.4768	0.6621
	H	0.2387	-2.2621	0.0291
	H	0.6000	-1.6832	1.5256
	O	-2.7243	-1.8018	-0.7680
	N	-1.7622	1.3752	0.5570
	H	-1.4095	2.2621	0.2078
	H	-2.7295	1.5439	0.8234
Y	C	0.5955	2.0577	-0.0597
	C	-0.3379	1.3041	0.9241
	C	0.3453	-1.0111	0.1458
	N	0.3166	1.6662	-1.4376
	H	0.4348	3.1299	0.1199
	H	-0.2224	1.7957	1.8970
	N	-0.0920	-0.1011	1.1692
	C	-0.0254	-2.4458	0.4969
	H	0.3450	-3.1299	-0.2685
	H	0.4142	-2.7314	1.4590
	H	-1.1090	-2.5473	0.5750
	H	-0.1077	-0.7025	-0.7929
	O	1.9516	1.8281	0.2509
	H	2.1028	0.8801	0.0697
	H	-0.6811	1.7458	-1.6093
	O	-1.6629	1.5060	0.4216
	H	0.3376	-0.2770	2.0675
	H	-2.2358	0.9212	0.9310
	O	1.7784	-0.9316	-0.1230
	H	0.7911	2.3055	-2.0675
	H	2.2358	-1.3771	0.6016
Z	C	0.9933	0.6944	1.0664
	C	1.4689	-0.7958	1.0602

	C	-0.9240	0.7488	-0.5321
	N	0.4243	1.1842	-0.1746
	H	0.2278	0.8182	1.8460
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	N	-0.9761	-0.7061	-0.8141
	C	-1.3874	1.5222	-1.7634
	H	-1.3232	2.5956	-1.5809
	H	-0.7554	1.2736	-2.6216
	H	-2.4205	1.2703	-2.0150
	H	-1.5688	1.0081	0.3181
	O	2.1491	1.4689	1.3629
	H	1.9046	2.3853	1.1849
	H	1.0662	0.9631	-0.9337
	H	-1.8050	-0.9395	-1.3522
	N	0.4257	-1.6346	1.6607
	H	0.7539	-2.5956	1.6874
	H	0.2504	-1.3538	2.6216
	O	1.7511	-1.2665	-0.2406
	H	-1.0135	-1.2218	0.0669
	H	0.9000	-1.2417	-0.7291
W	C	-0.8029	0.6801	0.5513
	C	-1.7685	-0.4731	0.9466
	C	0.8201	-0.2788	-1.1745
	N	0.5492	0.2905	0.1534
	H	-1.2423	1.2100	-0.3020
	H	-2.5874	-0.0297	1.5234
	N	0.5144	-1.7009	-1.3822
	C	2.2898	-0.0303	-1.5207
	H	2.5220	1.0348	-1.4750
	H	2.9369	-0.5501	-0.8048
	H	2.5182	-0.4077	-2.5195
	H	0.1907	0.2844	-1.8727
	H	1.0119	-0.2367	0.8885
	H	-0.4533	-1.8645	-1.1006
	N	-2.2272	-1.2122	-0.2234
	H	-2.9369	-1.8823	0.0571
	H	-2.6552	-0.5861	-0.8998
	O	-1.1422	-1.3737	1.8497
	H	1.1115	-2.2655	-0.7813
	H	-0.4854	-1.8652	1.3389
	N	-0.7718	1.5952	1.6936
	H	-0.5041	1.0625	2.5195
	H	-0.0234	2.2655	1.5402
U	C	0.2629	-0.9209	-0.2554
	C	-0.9289	-1.8494	0.0840
	C	-0.0410	1.4912	0.1098
	N	-0.1663	0.3803	-0.7861
	H	0.7889	-0.7355	0.6853
	H	-1.3274	-2.2564	-0.8593
	C	-0.5068	2.7846	-0.5416
	H	0.0828	2.9976	-1.4356
	H	-1.5606	2.6993	-0.8215
	H	-0.4051	3.6188	0.1554
	H	1.0098	1.5700	0.4105
	H	-1.1096	0.3317	-1.1590
	N	-0.4461	-2.8906	0.9890
	H	-1.1510	-3.6188	1.0638
	H	0.3757	-3.3171	0.5673
	O	-2.0160	-1.1580	0.6659
	H	-1.6577	-0.4309	1.2039

	O	-0.8281	1.2437	1.3204
	H	-0.4797	1.7812	2.0409
	N	1.1760	-1.6615	-1.1238
	H	0.7482	-1.7706	-2.0409
	H	2.0160	-1.1096	-1.2714
1	C	-1.9906	0.1615	0.2426
	C	-1.0965	-1.0256	-0.0170
	C	1.1270	-0.0718	-0.4076
	N	0.6788	1.2901	-0.0996
	H	-1.6746	-1.9548	0.0297
	N	0.1401	-1.1325	-0.2871
	C	2.3594	-0.5109	0.4048
	H	3.1701	0.2057	0.2573
	H	2.1095	-0.5391	1.4697
	H	2.6993	-1.5026	0.1012
	H	1.4000	-0.0836	-1.4697
	O	-3.1701	-0.0341	0.4568
	H	-1.5503	1.1649	0.2119
	H	1.3309	1.9548	-0.5049
	H	0.7065	1.4436	0.9066
2	C	1.6736	-0.7374	-0.2987
	C	1.6425	0.6588	0.3681
	C	-0.5125	0.1430	-0.3232
	N	0.2627	-1.0770	-0.5922
	H	2.2511	-0.6658	-1.2254
	H	2.3054	0.7030	1.2359
	N	0.2584	0.7966	0.7552
	C	-1.9459	-0.1464	0.0826
	H	-2.4621	-0.6991	-0.7059
	H	-1.9630	-0.7367	1.0034
	H	-2.4880	0.7857	0.2601
	H	-0.5061	0.7562	-1.2359
	O	2.2634	-1.6723	0.5844
	H	2.4880	-2.4605	0.0784
	H	0.0015	-1.7646	0.1125
	O	2.0833	1.5922	-0.6345
	H	-0.0074	1.7640	0.9131
	H	2.1433	2.4605	-0.2216
3	C	1.0413	0.6789	0.3608
	C	1.0027	-0.6888	-0.3289
	C	-1.1628	-0.1343	0.4683
	N	-0.3640	1.1118	0.3648
	H	1.3898	0.5446	1.3946
	H	0.9214	-0.4969	-1.4109
	N	-0.2534	-1.2801	0.1524
	C	-2.3736	-0.0945	-0.4561
	H	-2.9918	0.7836	-0.2482
	H	-2.0513	-0.0588	-1.5010
	H	-2.9826	-0.9897	-0.3156
	H	-1.5064	-0.2531	1.5010
	O	1.8767	1.5621	-0.3506
	H	2.0015	2.3567	0.1796
	H	-0.5283	1.5325	-0.5483
	H	-0.0217	-1.7620	1.0174
	N	2.1364	-1.5278	0.0280
	H	2.1489	-2.3567	-0.5595
	H	2.9918	-1.0201	-0.1828
4	C	-1.1482	-0.4184	-0.3779
	C	-1.1337	1.0004	0.2593
	C	1.0320	0.1893	0.3402

	N	0.2633	-0.8809	-0.3167
	H	-1.4583	-0.3309	-1.4229
	H	-1.3945	0.8902	1.3266
	N	0.2534	1.4081	0.0671
	C	2.4603	0.2865	-0.1658
	H	2.9888	-0.6567	-0.0064
	H	2.4607	0.5208	-1.2344
	H	3.0011	1.0764	0.3611
	H	1.0489	-0.0247	1.4229
	N	-2.0453	1.9902	-0.2968
	H	-3.0011	1.6673	-0.1714
	H	-1.8863	2.0539	-1.3000
	H	0.5024	2.1655	0.6972
	N	-2.1286	-1.2629	0.2896
	H	-1.8144	-1.4524	1.2389
	H	-2.1701	-2.1655	-0.1752
	H	0.6133	-0.9925	-1.2629
5	C	1.9384	-0.2373	0.4217
	C	0.8205	0.7968	0.1957
	C	-1.0882	-0.6169	-0.3454
	N	2.1314	-1.0423	-0.7988
	H	2.8406	0.3171	0.6968
	H	1.1475	1.8304	0.3363
	N	-0.4002	0.6409	-0.1108
	C	-2.3146	-0.6777	0.5599
	H	-2.8880	-1.5792	0.3390
	H	-1.9941	-0.7113	1.6044
	H	-2.9468	0.1980	0.4112
	H	-1.4116	-0.5617	-1.3943
	O	1.6805	-1.0881	1.5197
	H	0.8564	-1.5587	1.2970
	H	2.9468	-1.6374	-0.6783
	H	2.3053	-0.4468	-1.6044
	O	-0.3646	-1.8304	-0.1426
	H	0.4632	-1.7818	-0.6794
6	C	0.8282	-1.0773	-0.2899
	C	1.8945	-0.0221	-0.6012
	C	-1.2373	0.1628	-0.4143
	N	-0.4374	-1.0490	-0.1795
	H	1.2936	-2.0492	-0.0874
	H	2.5312	-0.4486	-1.3841
	N	-0.7825	1.2582	0.4730
	C	-2.7098	-0.1980	-0.2244
	H	-2.9970	-0.9955	-0.9142
	H	-2.8796	-0.5491	0.7976
	H	-3.3484	0.6696	-0.4105
	H	-1.0767	0.5084	-1.4413
	H	-1.4177	2.0492	0.3983
	N	2.7537	0.1757	0.5792
	H	2.1813	0.2825	1.4131
	H	3.3484	-0.6340	0.7317
	O	1.4093	1.1983	-1.0921
	H	0.7289	1.4970	-0.4415
	H	-0.8191	0.9464	1.4413
7	C	1.3080	-0.2011	-0.3876
	C	1.5867	1.0654	0.4224
	C	-1.2375	-0.3977	-0.1476
	N	-0.0153	-0.4720	-0.8967
	H	1.9433	-0.1144	-1.2821
	H	2.5931	1.0603	0.8544

	N	0.8520	2.0803	0.5982
	C	-1.1078	-0.8644	1.2974
	H	-0.7307	-1.8864	1.3387
	H	-0.4295	-0.2195	1.8560
	H	-2.0897	-0.8315	1.7752
	H	-1.9642	-1.0312	-0.6693
	O	1.7873	-1.2661	0.4378
	H	1.6316	-2.0803	-0.0551
	H	-0.1366	-0.1811	-1.8560
	O	-1.7444	0.9659	-0.2084
	H	-2.5931	0.9987	0.2501
	H	-0.0680	1.9388	0.1648
8	C	1.3309	-0.1936	-0.4142
	C	1.6023	1.0881	0.3761
	C	-1.2252	-0.4510	-0.1335
	N	0.0132	-0.5216	-0.8983
	H	1.9510	-0.1045	-1.3199
	H	2.6430	1.1319	0.7190
	N	0.8333	2.0599	0.6298
	C	-1.0555	-0.9134	1.3113
	H	-0.6209	-1.9120	1.3423
	H	-0.4052	-0.2365	1.8666
	H	-2.0305	-0.9378	1.8039
	H	-1.9088	-1.1491	-0.6348
	O	1.8588	-1.2348	0.4202
	H	1.6796	-2.0599	-0.0461
	H	-0.1153	-0.2647	-1.8666
	H	-0.1204	1.8685	0.2795
	N	-1.7987	0.9187	-0.1470
	H	-2.0874	1.1535	-1.0935
	H	-2.6430	0.9462	0.4204
9	C	-1.3941	-0.6154	0.3102
	C	-2.0462	0.7623	0.4104
	C	1.0272	-0.0016	0.2543
	N	-0.1276	-0.6073	-0.4143
	H	-1.2788	-0.9873	1.3441
	H	-3.0264	0.7192	0.9029
	N	-1.6332	1.8812	-0.0182
	C	2.2121	-0.9730	0.2522
	H	1.9775	-1.8812	0.8152
	H	2.4629	-1.2545	-0.7761
	H	3.0917	-0.5061	0.7007
	H	0.7728	0.2368	1.2956
	H	0.0672	-1.5692	-0.6645
	N	-2.2748	-1.5676	-0.3784
	H	-3.0917	-1.7681	0.1898
	H	-2.6085	-1.1555	-1.2464
	N	1.3237	1.2879	-0.3992
	H	2.0752	1.7646	0.0931
	H	1.6558	1.1078	-1.3441
	H	-0.6875	1.7880	-0.4180
10	C	-1.3996	-0.5742	0.2572
	C	-2.0259	0.8161	0.3346
	C	1.0214	-0.0149	0.2116
	N	-0.1295	-0.5715	-0.4586
	H	-1.2928	-0.9434	1.2908
	H	-2.9586	0.8346	0.9100
	N	-1.6308	1.8877	-0.2164
	C	2.2161	-0.9604	0.1598
	H	2.0008	-1.8877	0.6972

	H	2.4494	-1.1955	-0.8824
	H	3.0939	-0.4940	0.6117
	H	0.7717	0.2129	1.2578
	H	0.0419	-1.5081	-0.8007
	N	-2.2884	-1.5143	-0.4347
	H	-3.0939	-1.7310	0.1432
	H	-2.6380	-1.0912	-1.2908
	H	-0.7398	1.7196	-0.6972
	O	1.3465	1.2276	-0.4544
	H	1.9545	1.7173	0.1122
OH_PreIm	C	-1.4013	-0.2091	0.4526
	C	-0.8269	1.0804	-0.0983
	C	0.9504	-0.0934	0.5211
	N	-0.2346	-0.7320	1.1309
	H	-2.2423	-0.0686	1.1387
	H	-1.4488	1.8568	-0.5346
	N	0.4419	1.1363	-0.1025
	C	1.6768	-0.9513	-0.5184
	H	2.0697	-1.8568	-0.0488
	H	0.9792	-1.2379	-1.3085
	H	2.5113	-0.3999	-0.9576
	H	1.6536	0.1982	1.3085
	O	-1.8503	-0.9681	-0.6861
	H	-2.5113	-1.5984	-0.3805
	H	-0.2030	-1.7445	1.1257
NH2_PreIm	C	-1.2148	-0.2231	0.5195
	C	-0.6348	1.0552	-0.0608
	C	1.1697	-0.1102	0.5091
	N	0.0072	-0.8954	0.9817
	H	-1.8985	-0.0095	1.3496
	H	-1.2667	1.8450	-0.4620
	N	0.6326	1.1115	-0.1151
	C	2.0752	-0.8667	-0.4604
	H	2.4672	-1.7696	0.0148
	H	1.5148	-1.1560	-1.3539
	H	2.9188	-0.2418	-0.7616
	H	1.7675	0.2181	1.3687
	H	0.0204	-1.8450	0.6278
	N	-1.9636	-1.0330	-0.4467
	H	-2.9188	-0.6994	-0.5317
	H	-1.5387	-0.9737	-1.3687
OH_noncycPreIm	C	-0.9684	0.8884	-0.5641
	H	-1.3842	1.8330	-0.9245
	C	-2.0156	-0.0771	-0.1145
	H	-2.9622	0.3914	0.1730
	N	-1.8412	-1.3385	-0.0985
	H	-2.6705	-1.8330	0.2303
	N	0.2999	0.7876	-0.5534
	C	0.9625	-0.4389	-0.0482
	H	0.5531	-0.6626	0.9491
	O	0.7612	-1.5319	-0.9203
	H	-0.1710	-1.7936	-0.7778
	C	2.4542	-0.1802	0.0469
	H	2.6541	0.6756	0.6949
	H	2.9622	-1.0587	0.4495
	H	2.8493	0.0351	-0.9491
NH2_noncycPreIm	C	-2.0529	-0.2211	-0.4419
	C	-1.0479	-1.1272	0.2020
	C	0.9272	0.0649	-0.4132
	N	-2.0193	1.0483	-0.5199

	H	-2.9253	-0.7479	-0.8442
	H	-1.4952	-2.0020	0.6842
	N	0.2213	-1.0442	0.2474
	C	2.3676	-0.3736	-0.6739
	H	2.9253	0.4255	-1.1695
	H	2.8613	-0.6158	0.2713
	H	2.3908	-1.2594	-1.3143
	H	0.4484	0.3122	-1.3702
	N	0.8047	1.2605	0.4422
	H	-1.1615	1.4031	-0.0686
	H	1.1634	1.0453	1.3702
	H	1.3929	2.0020	0.0698
PreIm	C	-0.5834	-1.3914	0.7395
	C	-0.5834	-1.3914	-0.7395
	C	-0.5911	0.6649	0.0000
	N	-0.5886	-0.1905	1.1898
	H	-0.5794	-2.2662	1.3808
	H	-0.5794	-2.2662	-1.3808
	N	-0.5886	-0.1905	-1.1898
	C	0.5923	1.6356	0.0000
	H	0.5555	2.2662	0.8890
	H	1.5309	1.0769	0.0000
	H	0.5555	2.2662	-0.8890
	H	-1.5309	1.2324	0.0000
2MI	C	-1.5859	0.3504	-0.0001
	C	-1.5379	-1.0175	-0.0007
	C	0.5171	-0.3625	-0.0005
	N	-0.2677	0.7549	-0.0005
	H	-2.4019	1.0533	0.0000
	H	-2.3654	-1.7104	-0.0009
	N	-0.2265	-1.4543	0.0000
	C	2.0092	-0.3098	-0.0005
	H	2.3902	0.2126	-0.8830
	H	2.3902	0.2108	0.8830
	H	2.4019	-1.3259	-0.0015
	H	0.0563	1.7104	-0.0008

Table S10. Cartesian coordinates of the transition states with the participation of one water molecule

TS	**Atom**	**X**	**Y**	**Z**
GO+NH2NH2CHCH3_X	C	-2.1313	1.2791	-0.5787
	H	-2.0731	1.9593	-1.4540
	C	-1.3188	-0.0114	-0.7240
	H	-1.6191	-0.4422	-1.6997
	O	-1.4247	-0.8605	0.3199
	O	-2.8112	1.5376	0.3806
	O	0.6514	-1.9945	-0.1251
	H	1.2333	-2.0539	0.6392
	H	-0.4963	-1.5360	0.2315
	C	0.7975	1.4465	-0.1174
	C	0.7273	1.0712	1.3598
	H	1.1625	1.8830	1.9446
	H	-0.2990	0.8965	1.6804
	H	1.2977	0.1585	1.5429
	N	0.1695	0.3589	-0.9683
	H	0.3406	0.5958	-1.9446
	H	0.6516	-0.6154	-0.7298
	H	0.2256	2.3583	-0.3009
	N	2.1299	1.6422	-0.6513
	H	2.4124	2.6110	-0.5654

	H	2.8112	1.0752	-0.1564
	H	-0.9569	-1.6781	0.3114
	H	-0.0530	-2.6110	-0.2297
	H	-0.9939	-1.6473	-0.2363
	H	0.0437	-0.8679	-0.9430
Bc+OHNH2CHCH3_Y	C	-1.9178	-0.6610	-0.5905
	H	-1.9274	0.1892	-1.2846
	C	-0.6881	-0.5152	0.3308
	H	-0.6176	-1.4171	0.9531
	N	0.5325	-0.5022	-0.5949
	H	0.4089	-1.1953	-1.3359
	C	1.8369	-0.7151	0.1141
	H	1.8222	-0.0077	0.9465
	C	2.9828	-0.4331	-0.8362
	H	2.9142	0.5816	-1.2322
	H	3.9262	-0.5413	-0.3006
	H	2.9677	-1.1438	-1.6663
	O	-0.6898	0.6302	1.0734
	H	-0.4012	1.4418	0.2975
	O	0.0349	1.9985	-0.7762
	H	0.7763	2.5731	-0.5589
	H	0.4981	0.5307	-0.9664
	N	-3.0877	-0.7641	0.2525
	H	-3.0121	-0.0795	0.9999
	H	-3.9262	-0.5487	-0.2770
	O	-1.7966	-1.8145	-1.4205
	H	-2.0053	-2.5731	-0.8582
	O	1.9257	-2.0455	0.5562
	H	1.5184	-2.1242	1.4251
	H	0.0202	0.8083	1.6663
	H	-0.8297	0.9537	0.0588
	H	-0.2099	1.3033	-0.1896
	H	-0.0638	0.1366	-1.0553
Dc_Y	C	-1.0679	0.5698	0.4486
	C	-0.5636	-0.3006	-0.7234
	N	0.9328	-0.2263	-0.9036
	H	1.2239	0.8471	-0.9818
	H	1.1741	-0.7059	-1.7702
	C	1.6200	-2.0536	0.7763
	H	1.5728	-2.8069	-0.0116
	H	0.6745	-2.0410	1.3139
	H	2.4266	-2.3114	1.4657
	C	1.9259	-0.6809	0.2082
	H	2.8695	-0.7110	-0.3548
	O	1.9508	0.3020	1.1781
	O	1.8942	2.0837	-0.4430
	H	1.9954	1.2674	0.5730
	H	1.2905	2.8069	-0.2475
	H	-0.6797	1.5820	0.2854
	H	-0.9678	0.1393	-1.6389
	O	-1.0018	-1.6175	-0.5499
	H	-1.1318	-2.0279	-1.4115
	O	-0.6577	0.0898	1.7201
	H	0.3171	0.2176	1.7702
	N	-2.5052	0.6087	0.3491
	H	-2.8599	-0.3316	0.5060
	H	-2.8695	1.1903	1.0972
	H	1.3976	-0.6804	-0.1174
	H	0.7129	0.3910	-1.0802
	H	1.0980	-0.4100	-0.4845

	H	2.1314	1.1951	0.9391
	H	1.5655	1.2047	-0.5240
	H	1.4977	0.8506	0.3332
X_2	C	1.1953	-0.2840	0.7837
	H	0.8698	-0.3985	1.8263
	C	0.5615	-1.4434	-0.0334
	H	0.5970	-2.3822	0.5289
	O	1.2544	-1.5385	-1.2628
	O	2.5235	-0.0680	0.6762
	O	2.4699	1.5788	-1.0829
	H	2.6604	0.6615	-0.2046
	H	0.7319	-2.1214	-1.8263
	C	-0.8022	0.3696	-0.5579
	C	-2.1018	1.0762	-0.2303
	H	-2.0428	2.1342	-0.4916
	H	-2.9150	0.6242	-0.8003
	H	-2.3323	0.9881	0.8356
	N	-0.8249	-1.0607	-0.2660
	H	-1.3877	-1.2527	0.5584
	H	2.8702	2.3822	-0.7335
	H	-0.5448	0.5018	-1.6094
	N	0.3754	0.9289	0.2131
	H	1.1199	1.4319	-0.4342
	H	0.0854	1.5480	0.9656
	H	0.8160	0.6528	0.3174
	H	2.9150	0.0453	-0.1730
	H	1.6819	1.2380	-0.6953
	H	2.0719	0.3403	-0.3757
	H	0.9037	0.1532	0.6123
	H	0.6321	0.9708	-0.6025
Y_2	C	0.6913	1.7261	-0.5025
	C	1.1789	0.8318	0.7024
	C	-1.2031	0.3886	-1.2109
	H	-0.0058	2.4708	-0.1205
	H	1.4604	1.5441	1.4921
	N	-0.0097	0.8323	-1.4249
	H	0.6327	0.1938	-1.9410
	N	0.2240	-0.1027	1.0556
	H	0.1952	-1.4841	0.3100
	C	-2.2968	1.0431	-0.4550
	H	-1.9789	1.8877	0.1474
	O	2.4686	0.1995	0.2590
	H	3.0562	0.9184	-0.0140
	O	1.7915	2.3179	-1.1377
	H	1.4935	3.0755	-1.6533
	H	-1.4628	-0.5050	-1.7714
	H	0.1912	-0.1962	2.0656
	O	0.1704	-2.3782	-0.2428
	H	-0.7626	-2.5588	-0.3939
	O	1.7575	-1.1870	-2.0656
	H	1.1566	-1.7950	-1.5711
	H	2.2401	-0.7750	-1.3198
	H	-2.7681	0.3026	0.1923
	H	-3.0562	1.3659	-1.1790
	H	0.4623	-1.0033	0.6402
	H	-0.3447	-1.6626	-0.0844
	H	0.7496	-3.0755	0.0136
2_OH_PreIm	C	1.3437	-1.3548	0.3046
	H	1.9341	-1.6166	1.1926
	C	0.0731	-0.6678	0.7633

	H	-0.5833	-1.0782	1.5157
	O	-1.3795	-1.1676	-0.6942
	O	1.0452	-2.5316	-0.4173
	H	1.8688	-3.0252	-0.4973
	H	-1.8677	-1.9232	-0.3495
	C	1.1566	0.8818	-0.5009
	C	1.9095	2.1766	-0.2521
	H	2.6725	2.3202	-1.0204
	H	1.2236	3.0252	-0.2866
	H	2.3902	2.1530	0.7296
	N	0.1341	0.6167	0.5404
	H	-0.8537	1.0753	0.4430
	H	0.6232	0.9391	-1.4574
	N	2.0159	-0.3076	-0.4637
	H	2.9105	-0.0808	-0.0472
	O	-2.3086	0.9835	-0.0658
	H	-2.3829	1.5296	-0.8558
	H	-1.9436	-0.1985	-0.4489
	H	-1.6295	-0.7803	-1.5157
	H	-1.0755	0.4806	0.1674
	H	-2.9105	0.2723	0.0735
	H	-2.0439	-0.8434	-0.6790
5_OH_PreIm (with the participation of two water molecules)	C	0.7449	1.0839	0.3483
	C	0.7027	2.3147	1.2009
	H	1.4924	2.9838	0.8639
	H	-0.2635	2.8143	1.1106
	H	0.8846	2.0495	2.2424
	H	-0.5462	-0.8832	1.4238
	O	0.6355	-2.2833	0.3890
	H	1.4996	-1.8798	0.1172
	H	0.8797	-2.9838	1.0022
	H	1.3170	0.2242	0.6371
	O	2.8934	1.3861	-0.3461
	H	2.6203	1.6226	-1.2390
	O	3.0043	-1.0923	-0.2014
	H	3.0052	-0.0210	-0.3223
	H	3.5474	-1.2438	0.5794
	N	-0.9592	-0.0155	1.0905
	H	-1.5336	0.4538	1.7813
	N	0.2206	1.1372	-0.9179
	C	-1.6487	-0.2054	-0.1759
	H	-1.6013	-1.2652	-0.4509
	C	-0.8623	0.5674	-1.2250
	H	-1.2425	0.6064	-2.2424
	O	-2.9655	0.2955	-0.1820
	H	-3.5474	-0.3732	0.1966
	H	2.4561	0.6880	0.1108
	H	2.2745	-1.6590	-0.3847
	H	2.3960	-0.2965	-0.5008
OH_PreIm_PreIm	C	-0.5955	0.4607	0.7339
	H	-1.3362	0.6566	1.4913
	C	0.3523	1.4123	0.1320
	H	0.3090	2.4882	0.2458
	O	-2.2488	0.5883	-0.6990
	H	-2.9596	1.0657	-0.2550
	C	0.9439	-0.6163	-0.5047
	C	2.1692	-1.4294	-0.0978
	H	1.9120	-2.4882	-0.0452
	H	2.9618	-1.2929	-0.8344
	H	2.5274	-1.1008	0.8797

	N	1.2270	0.8114	-0.5828
	H	-2.9618	-1.9219	0.5397
	H	0.5860	-0.9365	-1.4913
	N	-0.1626	-0.7454	0.4585
	H	-0.9718	-1.4773	0.3314
	O	-2.3702	-1.7803	-0.2077
	H	-2.4276	-0.5804	-0.4924
	H	-2.3828	-0.3004	-0.9810
	H	-1.4497	-1.7200	-0.1063
	H	-2.4457	-2.3189	-0.9768
	H	-2.5942	-1.1754	-0.8039
PreIm_2MI	C	1.5645	0.8964	-0.6909
	H	2.4092	0.8003	-1.3601
	C	1.5549	1.1075	0.6886
	H	2.3959	1.2250	1.3601
	O	0.0183	-1.7709	0.1709
	H	0.4023	-1.8373	1.0617
	C	-0.4670	0.8768	0.0157
	C	-1.9632	1.0332	-0.0134
	H	-2.3945	0.4862	-0.8546
	N	0.2751	1.1012	1.1400
	H	-0.2023	-0.7208	-0.0283
	N	0.2840	0.7562	-1.1290
	H	0.6732	-2.0862	-0.4743
	H	-2.2473	2.0862	-0.1217
	H	-2.4092	0.6641	0.9128